



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 12:07 PM UTC

PDB ID : 7K5B / pdb_00007k5b
EMDB ID : EMD-22679
Title : Structure of outer-arm dynein bound to microtubule doublet in microtubule binding state 2 (MTBS-2)
Authors : Rao, Q.; Zhang, K.
Deposited on : 2020-09-16
Resolution : 4.50 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

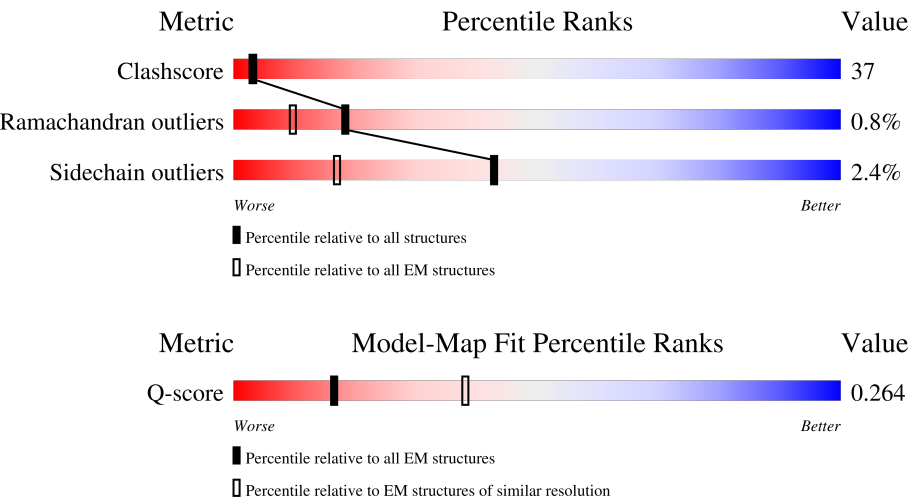
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4615	
2	B	4588	
3	C	3947	
4	D	595	

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Mol	Chain	Length	Quality of chain
5	E	557	
6	F	128	
7	G	151	
8	H	91	
9	I	106	
10	J	95	
11	K	90	
12	L	111	
13	M	87	
14	N	114	
15	O	120	
16	P	112	
17	Q	192	
18	R	150	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	ADP	A	4701	-	-	X	-
19	ADP	A	4901	-	-	X	-
19	ADP	B	5501	-	-	X	-
19	ADP	C	4702	-	-	X	-
20	ATP	A	4801	-	-	X	-
20	ATP	B	5601	-	-	X	-
21	MG	A	5002	-	-	X	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 119573 atoms, of which 156 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dynein heavy chain, outer arm protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4453	Total	C	N	O	S	0	0
			33975	21575	5802	6440	158		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3238	ASN	ASP	conflict	UNP Q22A67

- Molecule 2 is a protein called Outer arm dynein beta heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4524	Total	C	N	O	S	0	0
			34751	22080	5950	6571	150		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	36	ALA	GLN	conflict	UNP I7M9J2
B	1287	ALA	LEU	conflict	UNP I7M9J2
B	3977	ALA	SER	conflict	UNP I7M9J2

- Molecule 3 is a protein called gamma heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	3947	Total	C	N	O	S	0	0
			30427	19395	5159	5724	149		

- Molecule 4 is a protein called Dynein intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	579	Total	C	N	O	S	0	0
			4680	2975	791	883	31		

- Molecule 5 is a protein called Flagellar outer dynein arm intermediate protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	555	Total	C	N	O	S	0	0
			4440	2798	762	858	22		

- Molecule 6 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	128	Total	C	N	O	S	0	0
			996	625	176	193	2		

- Molecule 7 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	151	Total	C	N	O	S	0	0
			1024	636	184	203	1		

- Molecule 8 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	91	Total	C	N	O	S	0	0
			750	483	124	139	4		

- Molecule 9 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	106	Total	C	N	O	S	0	0
			827	526	134	161	6		

- Molecule 10 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	95	Total	C	N	O	S	0	0
			807	527	135	140	5		

- Molecule 11 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	90	Total	C	N	O	S	0	0
			754	489	124	137	4		

- Molecule 12 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	111	Total	C	N	O	S	0	0
			855	555	145	152	3		

- Molecule 13 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	87	Total	C	N	O	S	0	0
			735	477	123	130	5		

- Molecule 14 is a protein called Dynein light chain tctex-type 1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	114	Total	C	N	O	S	0	0
			852	542	142	165	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	92	ALA	ASN	conflict	UNP A4VEB3

- Molecule 15 is a protein called Dynein light chain 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	120	Total	C	N	O	S	0	0
			994	639	173	179	3		

- Molecule 16 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	109	Total	C	N	O	0	0
			541	323	109	109		

- Molecule 17 is a protein called Dynein light chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	192	Total	C	N	O	0	0
			1006	610	203	193		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	2	ALA	SER	conflict	UNP Q1HGH9

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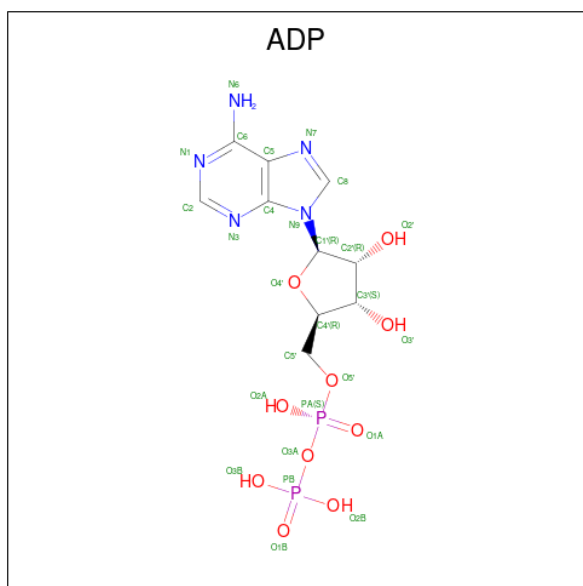
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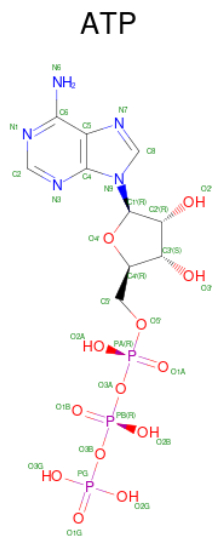
Chain	Residue	Modelled	Actual	Comment	Reference
Q	179	MET	TYR	conflict	UNP Q1HGH9

- Molecule 18 is a protein called Dynein light chain 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	150	Total	C	H	N	O	0	0
			895	439	156	150	150		

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).





Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total 31	C 10	N 5	O 13	P 3	0
20	B	1	Total 31	C 10	N 5	O 13	P 3	0
20	C	1	Total 31	C 10	N 5	O 13	P 3	0

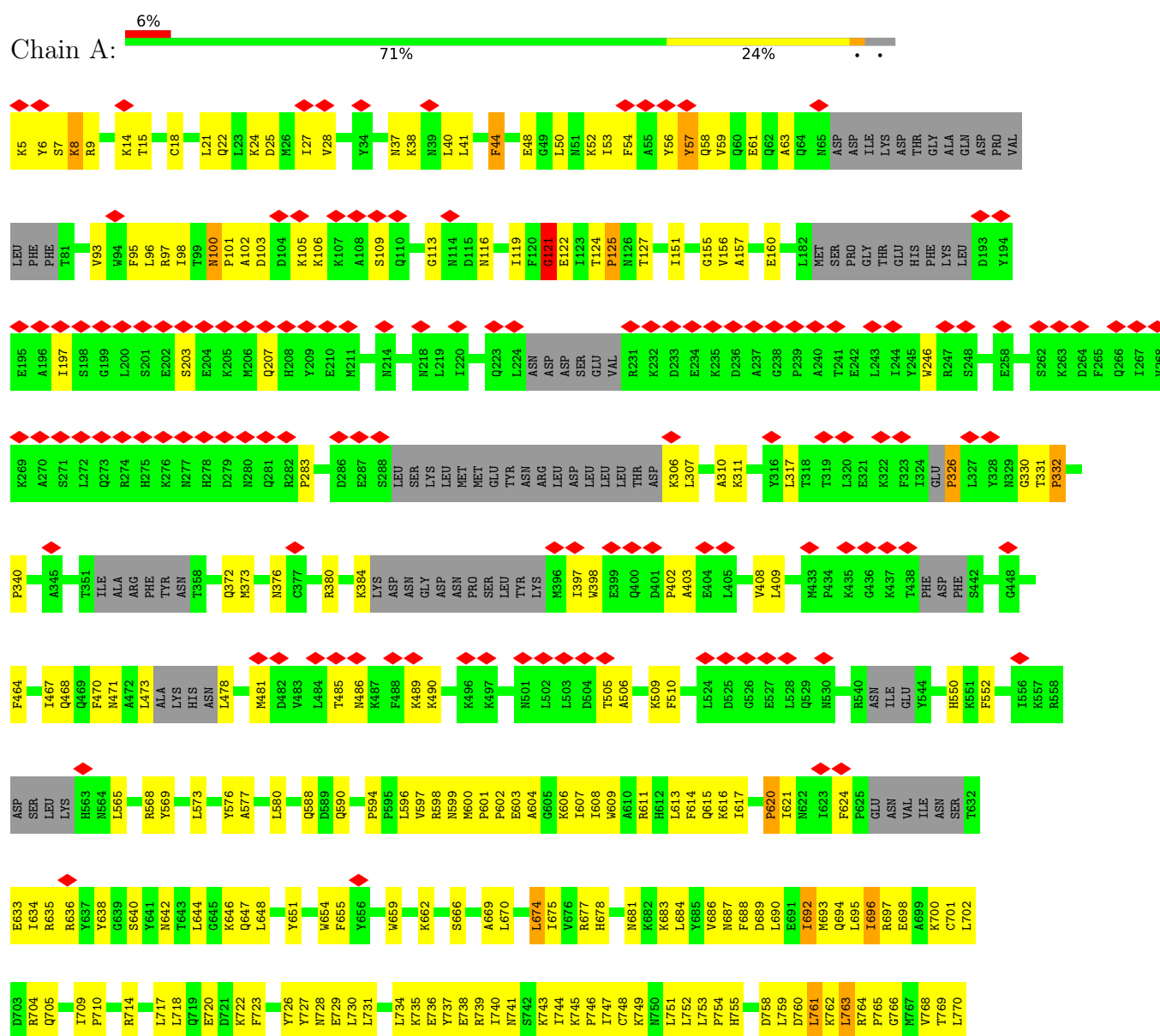
- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
21	A	3	Total Mg 3 3	0
21	B	3	Total Mg 3 3	0
21	C	3	Total Mg 3 3	0

3 Residue-property plots

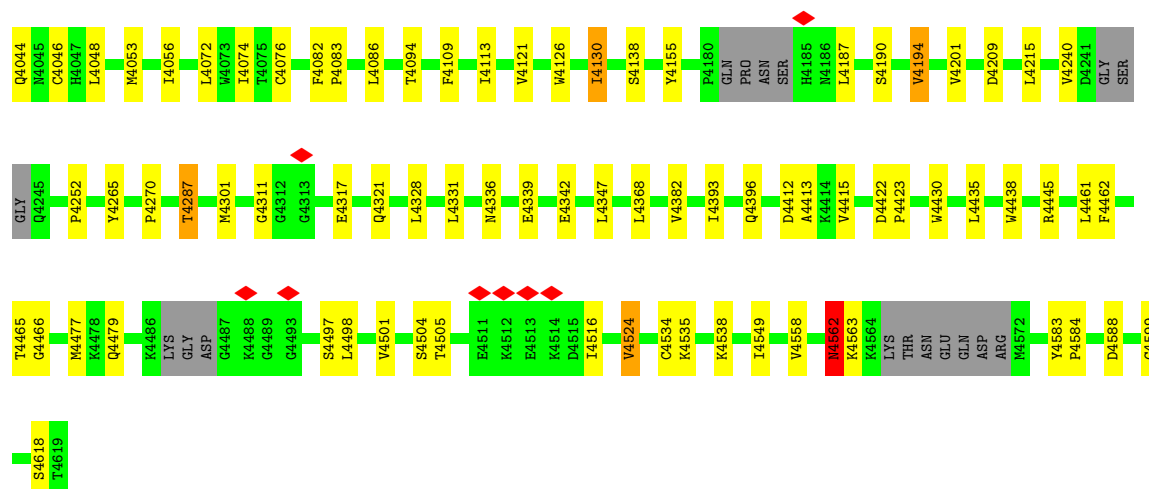
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Dynein heavy chain, outer arm protein



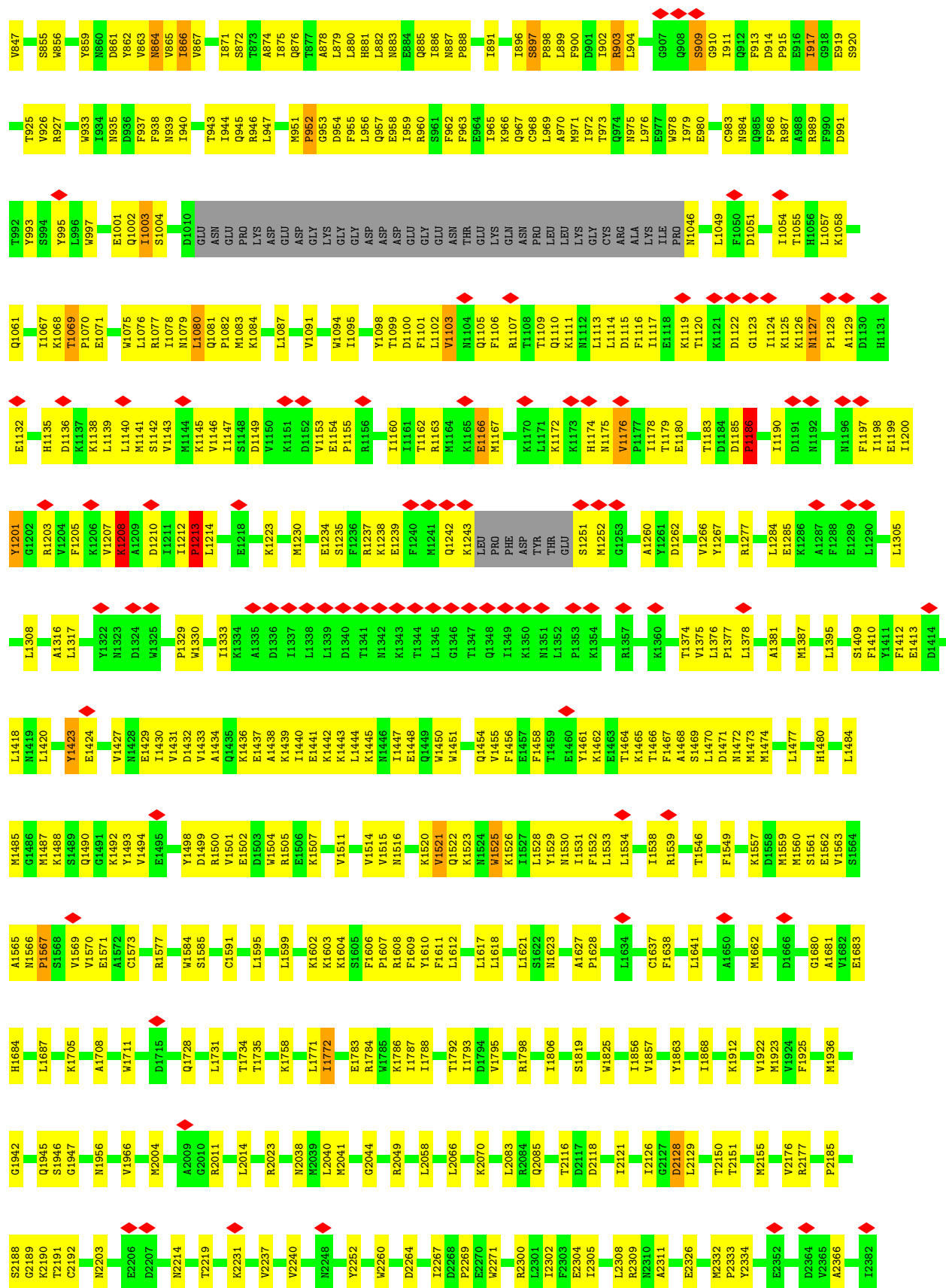
L1825	K1645	K1580	W1511	D1434	K1342	K1217	Y1134	Q1051	LYS	GLY	T845	T771
T1828	K1646	L1581	V1512	E1435	D1343	K1216	V1135	L1052	ASP	LYS	D846	W772
D1829	P1647	E1582	V1513	I1436	L1344	M1246	M1136	L052	THR	LYS	F847	S773
W1830	P1648	K1585	K1514	W1440	Q1348	VAL	E1137	E1059	GLY	PRO	T849	S774
D1831	A1649	K1586	K1515	N1441	A1349	GLY	T1138	E1060	LYS	ALA	S850	I777
S1832	Q1652	M1587	L1517	D1442	A1349	GLY	L1139	E1061	ASP	ASN	K851	Y780
F1838	T1653	L1588	W1518	M1443	N1355	ILE	E1140	I1062	T984	THR	N852	L781
L1839	T1654	T1589	T1519	Q1444	N1355	SER	Q1141	E1063	F985	LEU	V853	L781
L1840	Q1655	S1520	S1520	F1445	N1355	PRO	R1143	E1063	Y986	GLN	E854	
K1842	Q1657	F1446	E1522	Q1446	I1368	ALA	Q1146	V1066	I989	ASN	A858	G787
L1845	K1675	F1447	P1523	F1447	SER	GLY	Q1146	P1067		LEU	L788	K789
C1846	E1676	G1448	W1524	G1448	LEU	ALA	I1149	T1068	D992	LYS	V859	K790
I1847	E1677	I1449	F1525	I1449	LYS	MET	D1150	Y1069	K993	PRO	D860	K790
I1856	G1678	W1450	G1528	W1450	LYS	E1247	M1151	K1070	E994	LYS	D861	L791
Q1860	N1679	K1452	G1528	K1452	PRO	Y1280	F1152	G1072	Y995	F930	L862	E792
A1861	I1680	R1453	G1528	R1453	SER	Y1263	F1153	A1073	Y996	Q932	Q793	E793
M1862	E1681	ASP	E1522	ASP	ILE	Y1264	N1154	E1074	K997	V935	M867	L794
G1868	D1682	VAL	E1522	VAL	MET	I1265	P1155	E1075	V998	V936	L868	I795
L1869	W1683	CYS	E1522	CYS	P1377	I1265	Q1157	L1076	S1005	Q936	M869	D800
L1870	L1684	M1458	E1522	M1458	R1378	R1268	E1159	M1077	Q1007	L937	L871	I801
E1880	L1687	L1459	Q1540	L1459	K1390	G1269	M1159	T1078	G1008	N938	D872	E803
L1889	E1687	N1460	F1541	N1460	L1391	E1270	L1162	C1082	T1009	G939	P873	N804
F1892	L1689	G1461	I1544	G1461	N1392	N1271	L1163		K1010	D940	H874	R805
T1896	L1711	V1464	D1545	V1464	Y1393	L1272	Y1166	S1086	M1011	N942	V875	I806
K1909	S1720	I1467	W1548	I1467	E1394	G1273	Q1157	T1087	K1012	Y943	E807	N808
I1910	L1727	L1468	M1549	L1468	N1395	G1274	E1167	W1088	V1013	L944	L879	K811
L1914	N1745	D1474	K1550	D1474	P1396	Q1276	T1171	E1091	F1016	N945	P880	T812
V1915	K1758	L1478	M1551	L1478	D1397	N1277	T1172	K1093	L1017	PRO	E882	V813
Q1916	L1764	F1481	M1552	F1481	Y1400	Y1280	E1176	L1094	F1020	SER	T883	S814
G1918	L1778	N1482	E1553	N1482	I1404	P1281	R1180	Q1095	T1021	Q949	I886	K815
L1919	R1778	S1483	A1554	S1483	M1405	E1282	S1181	Y1096	F1023	Q952	K887	V816
W1920	T1779	Q1484	A1555	Q1484	G1406	L1283	L1182		E1024	I951	L818	V817
D1924	K1780	H1486	V1556	H1486	A1407	E1284	L1183	L1100	W1025	Q952	V819	W820
F1923	I1787	V1487	V1557	V1487	K1285	K1285	W1187	L1111	L1026	I955	H820	L821
C1922	Q1788	P1488	T1568	P1488	A1288	A1288	L1190	Q1114	C1027	A958	P822	P822
F1926	H1789	F1490	K1563	F1490	E1289	E1289	L1191	T1115	K1028	A959	GLN	ASP
L1934	Q1791	F1491	C1564	F1491	I1290	I1290	K1199	T1116	T960	L969	THR	LYS
S1935	T1792	A1491	C1565	A1491	K1291	K1291	Y1201	M1117	S1030	A961	LYS	PRO
L1935	D1793	E1493	M1569	E1493	E1414	E1414	Q1200	L1118	I1031	V962	LEU	LEU
I1962	T1794	V1494	V1570	V1494	D1415	D1415	Q1202	L1121	Q1032	L963	S901	SER
L1967	F1806	T1500	F1573	T1500	S1422	S1422	H1203	K1121	E1033	C965	L830	L830
V1970	Q1809	V1504	L1574	V1504	Q1426	Q1426	K1204	K1124	S1034	S966	D831	D831
F1973	T1814	N1505	L1577	N1505	L1427	L1427	Q1205	P1125	K1037	K967	S832	S832
		D1644	N1578	D1509	ASP	ASP	A1206	Y1126	N1041	H968	N907	N907
			E1579	P1510	L1323	L1323	Y1207	K1127	G1042	L969	A908	A908
					D1329	D1329	Y1208	K1127	P1043	Y970	M909	M909
					S1338	S1338	L1209	K1127	T1044	W972	K910	K910
					R1339	R1339	E1210	D1130	T1045	D973	Y911	Y911
					L1340	L1340	E1211	S1131	Q1046	Q974	R912	R912
					L1432	L1432	L1212	L1132	GLN	GLN	V913	V913
					L1433	L1433	K1213	G1133	ASN	ASN	CYS	CYS

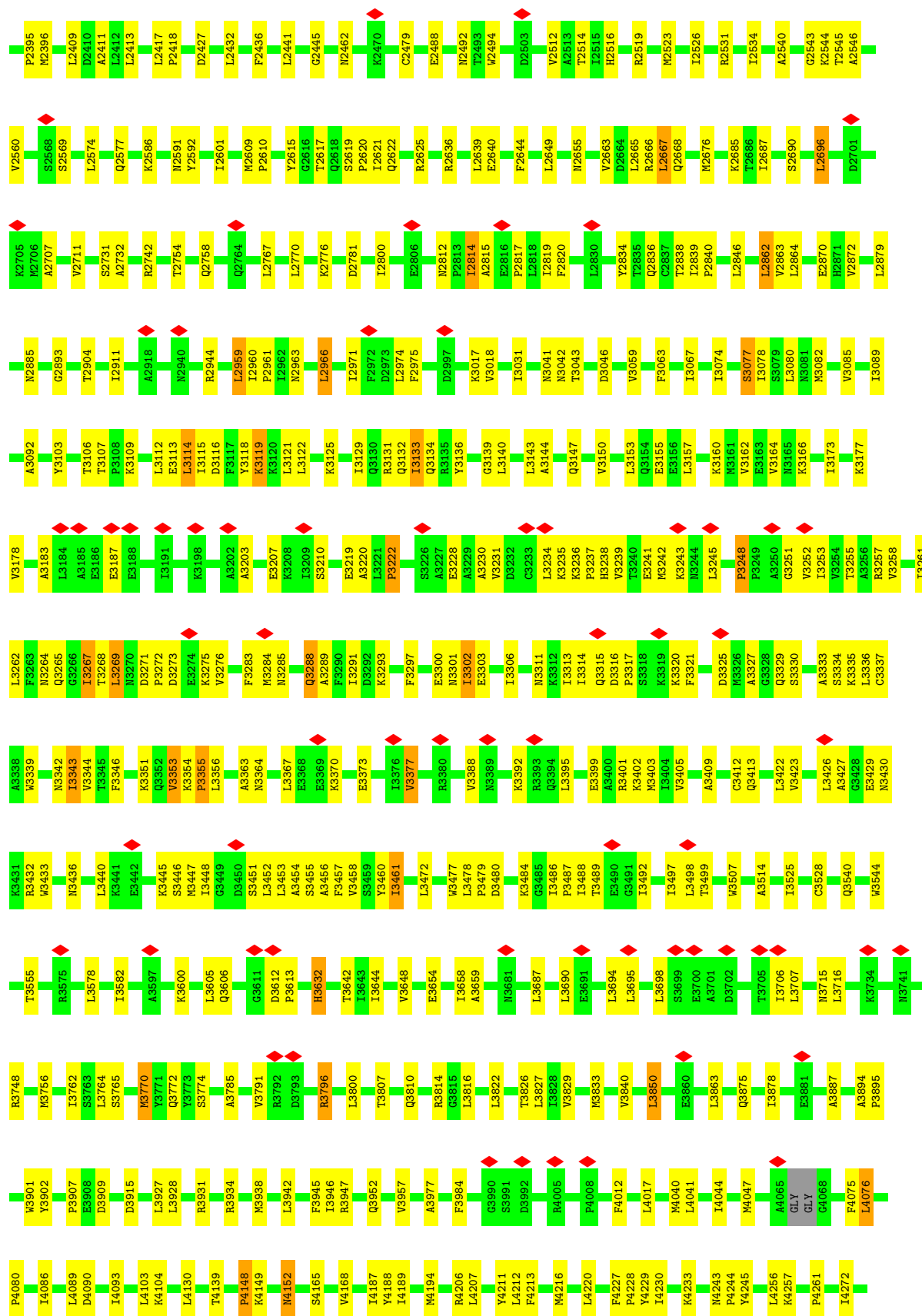


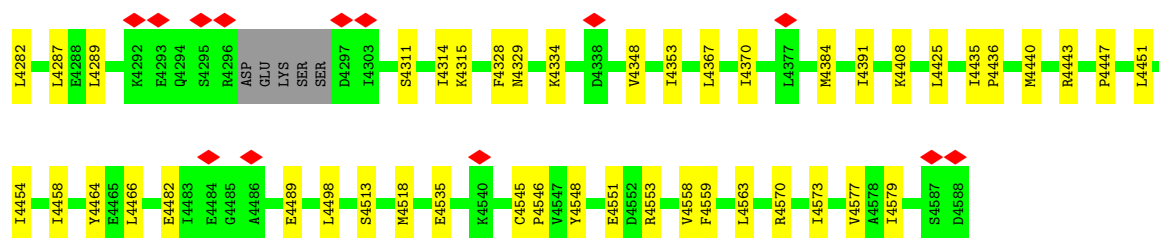


• Molecule 2: Outer arm dynein beta heavy chain

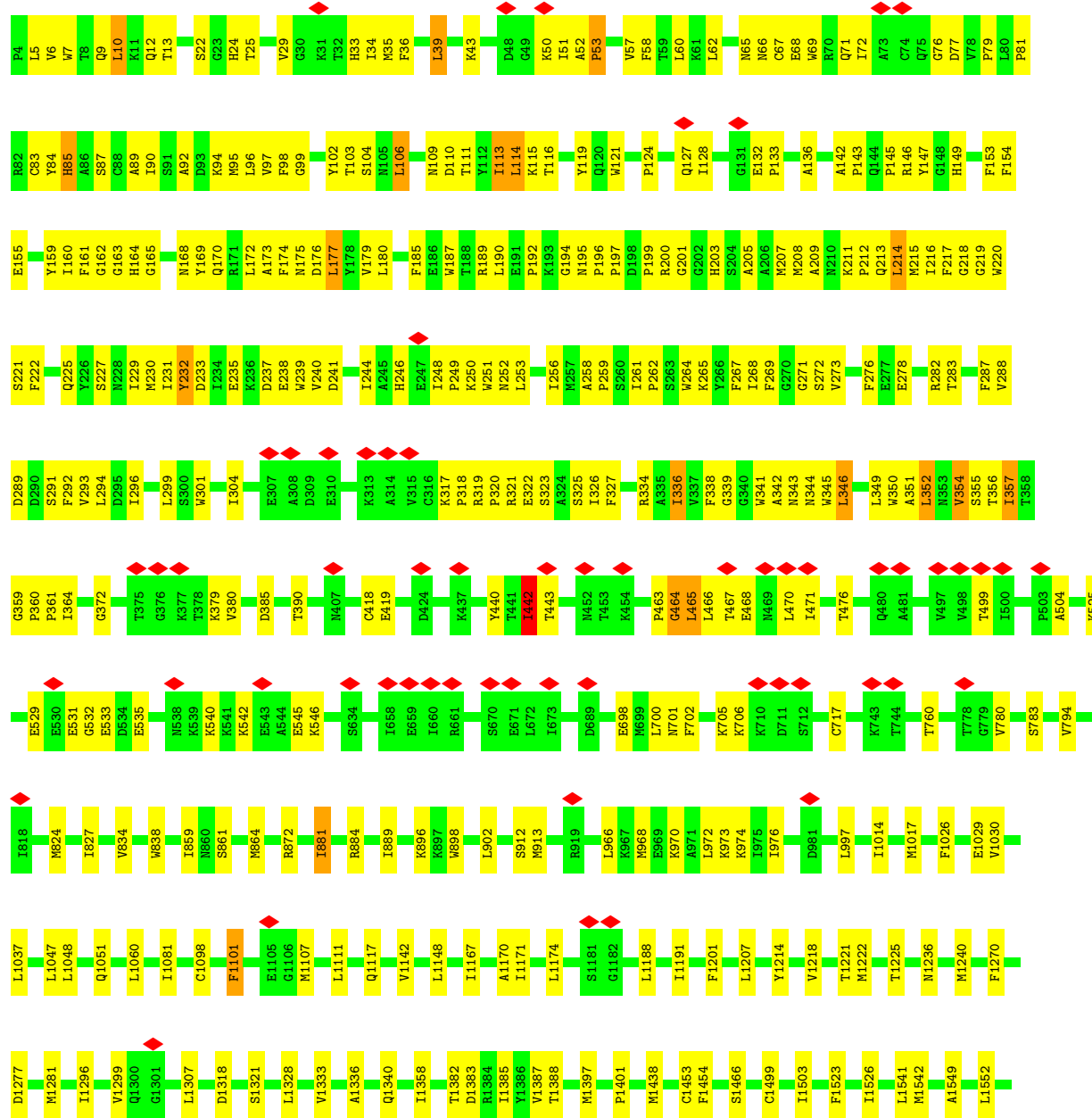
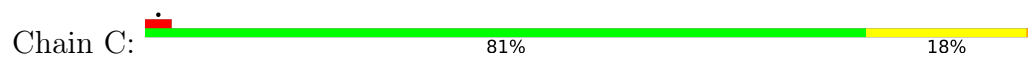


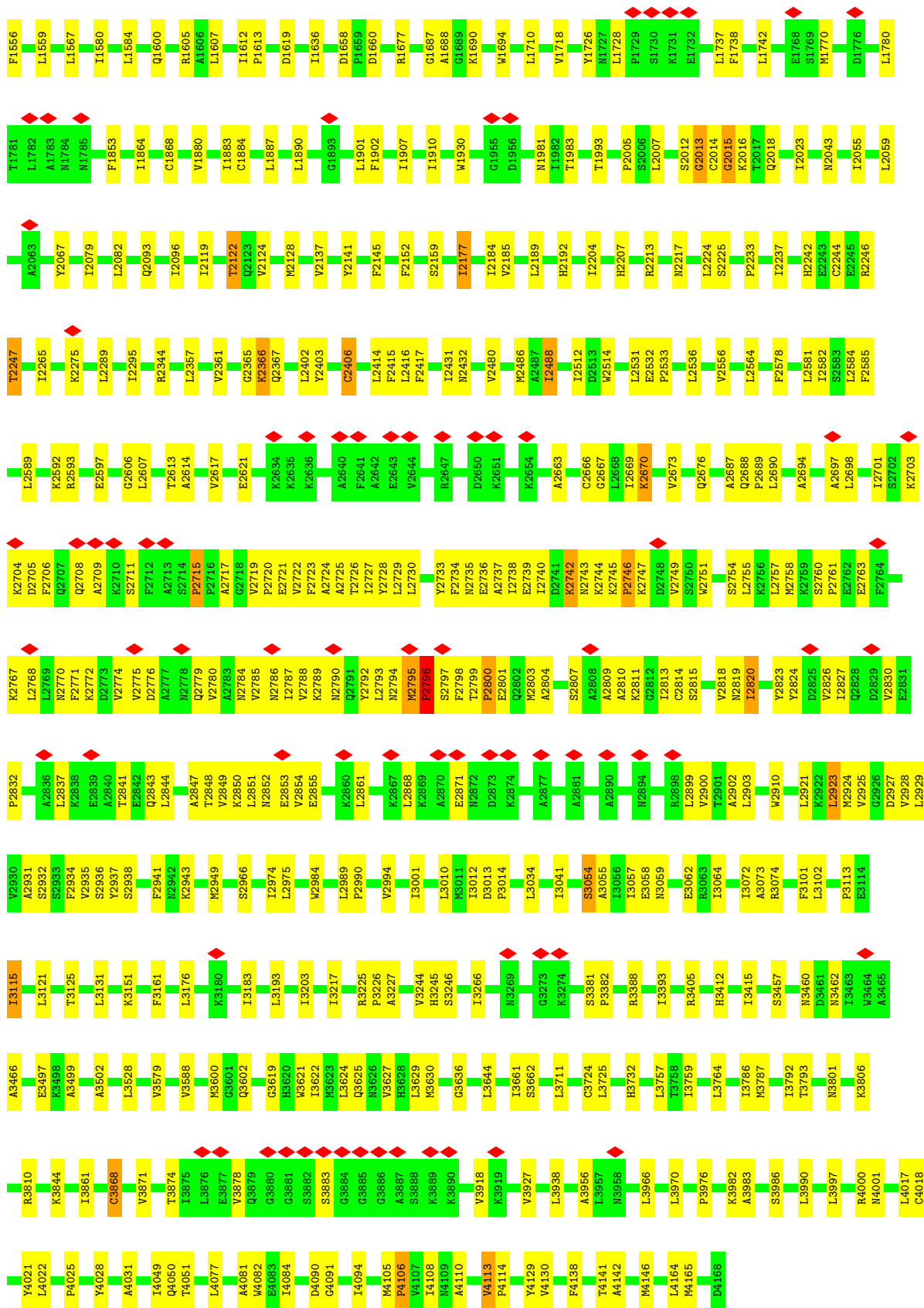




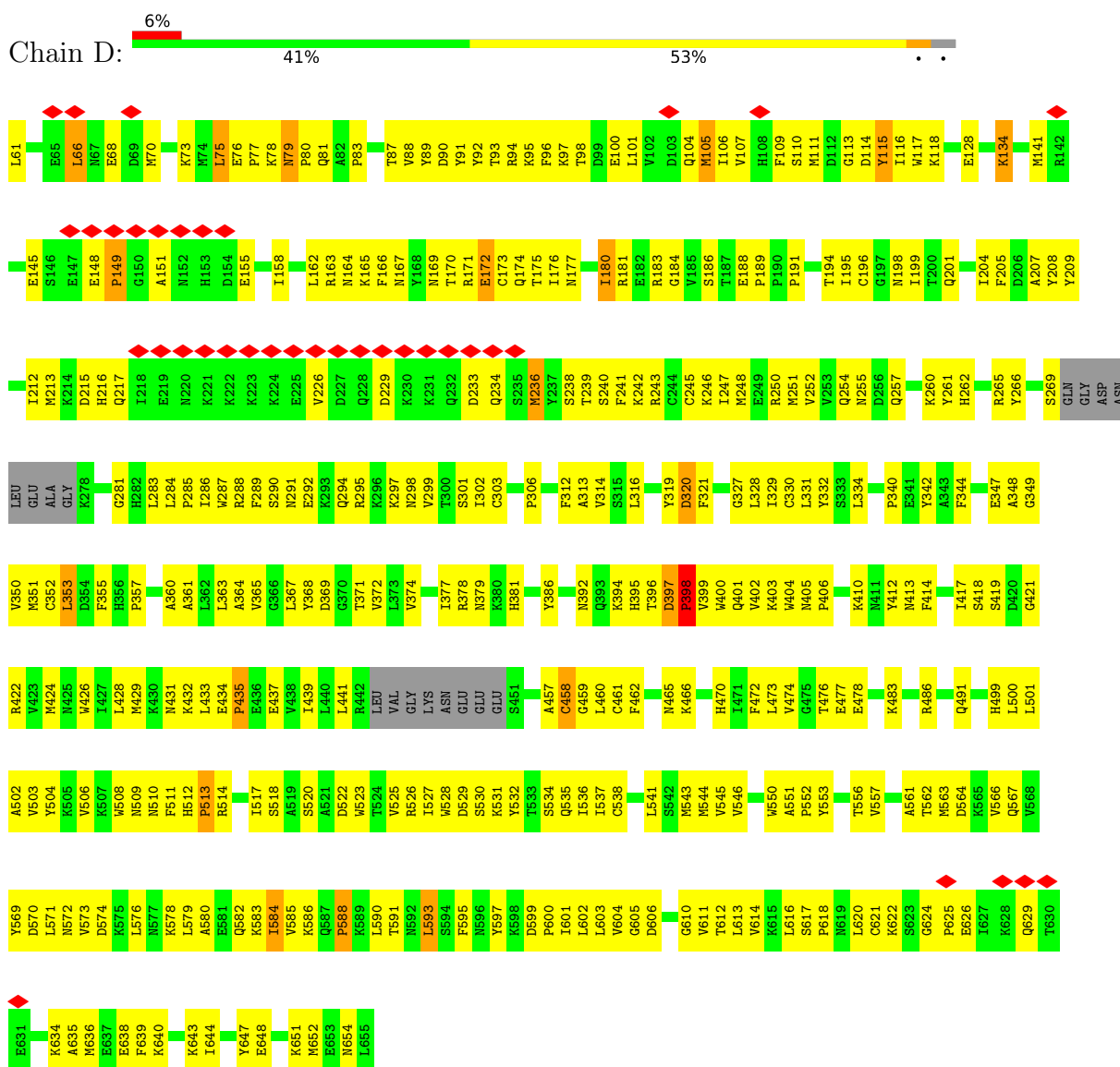


• Molecule 3: gamma heavy chain

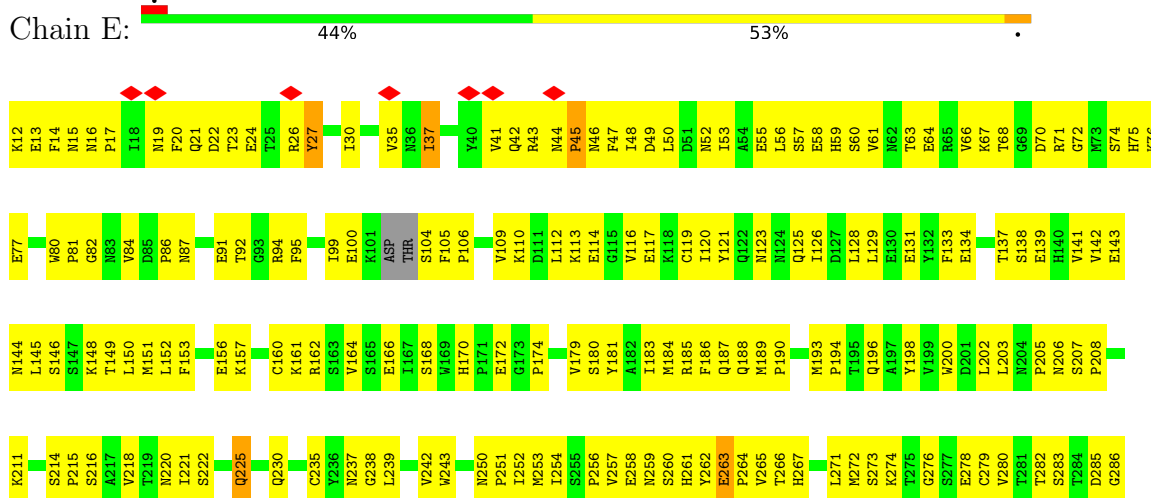


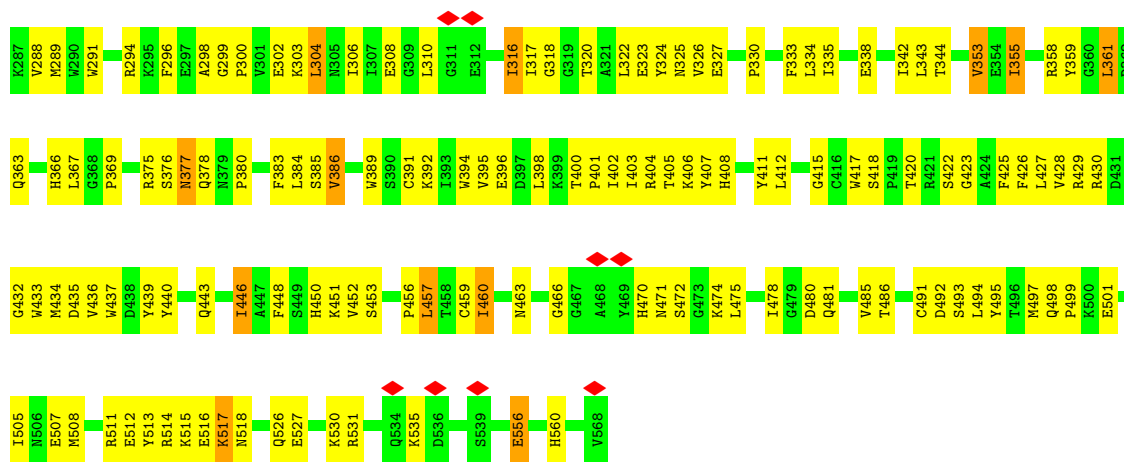


- Molecule 4: Dynein intermediate chain 2

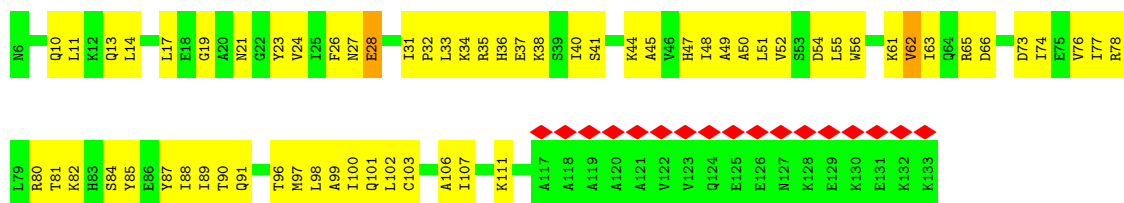


• Molecule 5: Flagellar outer dynein arm intermediate protein, putative

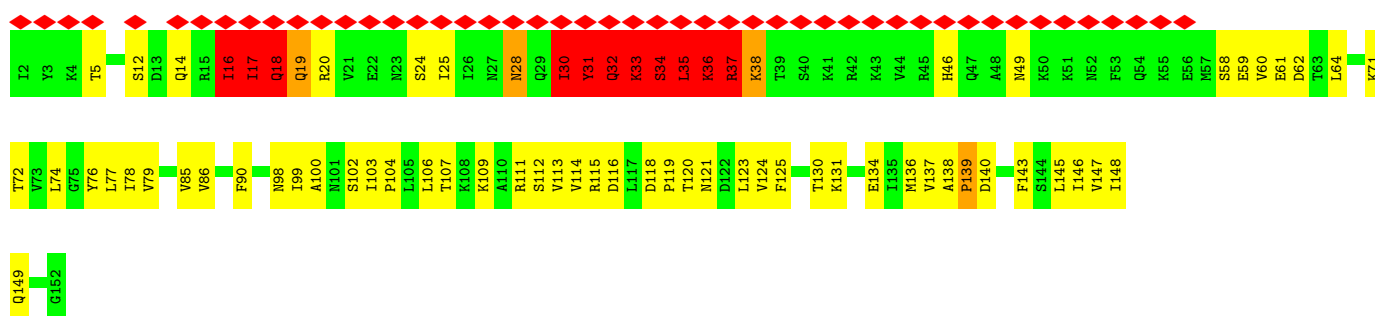




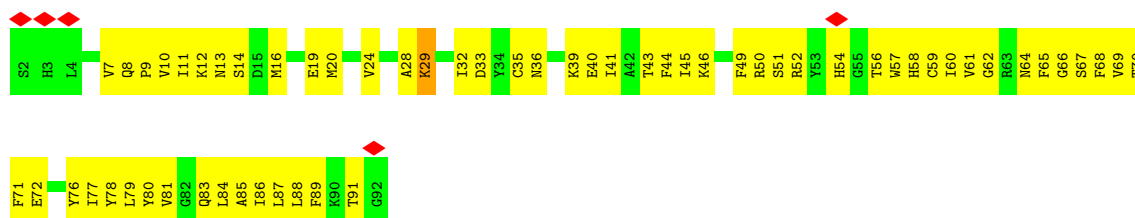
• Molecule 6: Dynein light chain roadblock-type 2 protein



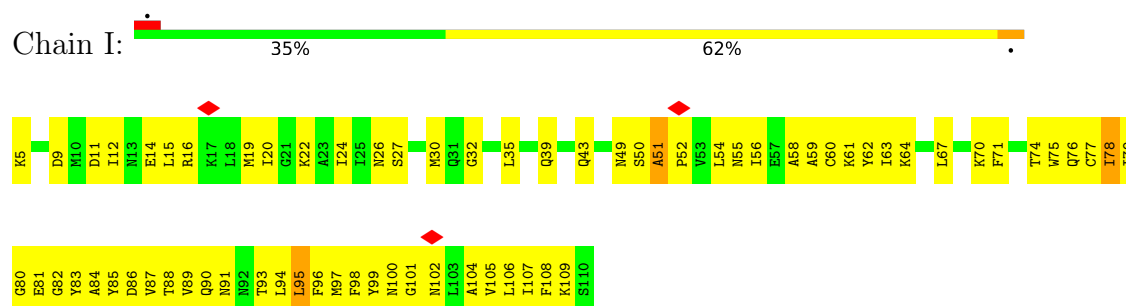
• Molecule 7: Dynein light chain roadblock-type 2 protein



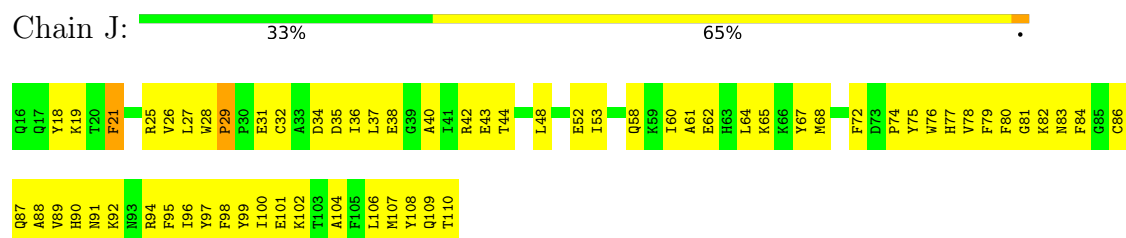
• Molecule 8: Dynein light chain



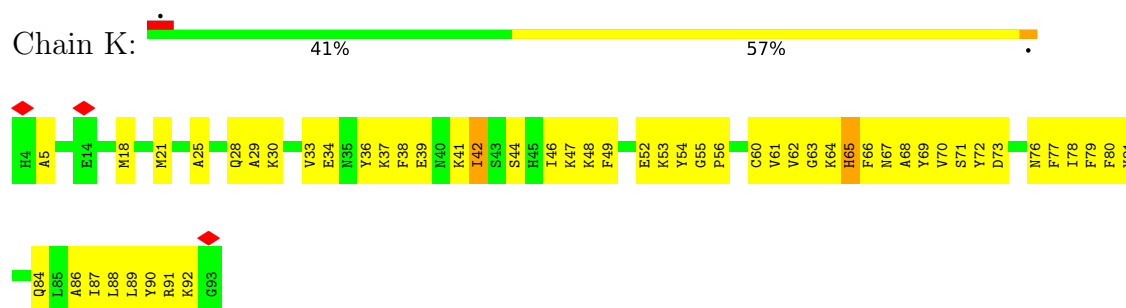
- Molecule 9: Dynein light chain



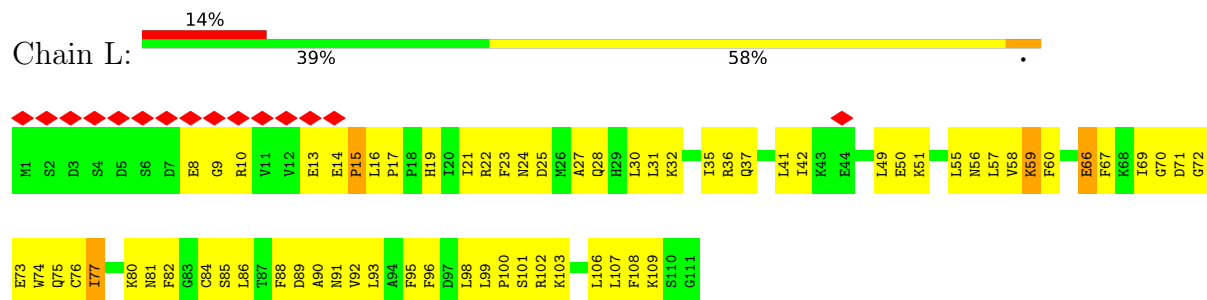
- Molecule 10: Dynein light chain



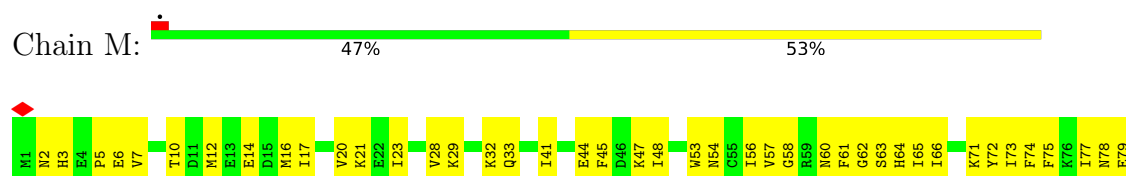
- Molecule 11: Dynein light chain



- Molecule 12: Dynein light chain

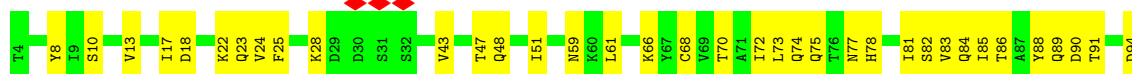


- Molecule 13: Dynein light chain





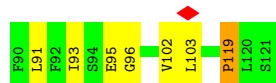
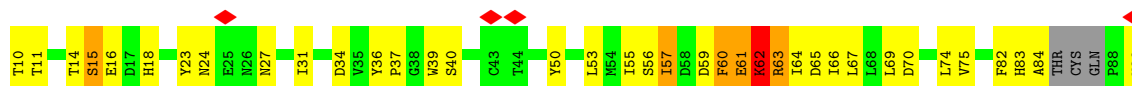
- Molecule 14: Dynein light chain tctex-type 1 protein



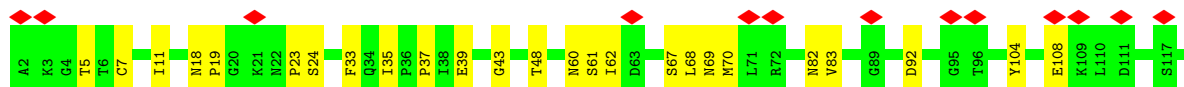
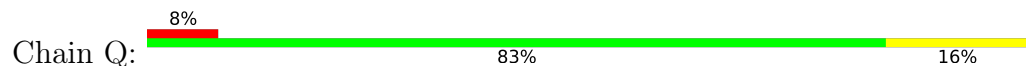
- Molecule 15: Dynein light chain 2A



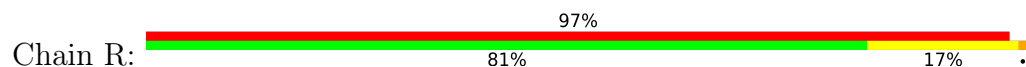
- Molecule 16: Thioredoxin



- Molecule 17: Dynein light chain 1



- Molecule 18: Dynein light chain 4A



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76936	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	8.594	Depositor
Minimum map value	0.000	Depositor
Average map value	0.029	Depositor
Map value standard deviation	0.189	Depositor
Recommended contour level	0.7	Depositor
Map size ($\text{\AA}$)	527.86786, 493.20984, 462.55084	wwPDB
Map dimensions	396, 370, 347	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3329996, 1.3329996, 1.3329996	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.04	14/34544 (0.0%)	1.54	57/46728 (0.1%)
2	B	1.11	18/35358 (0.1%)	1.61	86/47850 (0.2%)
3	C	1.02	2/31033 (0.0%)	1.57	48/42007 (0.1%)
4	D	0.98	1/4789 (0.0%)	1.27	10/6477 (0.2%)
5	E	0.94	0/4540	1.18	3/6136 (0.0%)
6	F	0.87	0/1008	1.06	0/1355
7	G	0.95	0/1030	1.67	14/1403 (1.0%)
8	H	0.98	0/767	1.13	0/1031
9	I	1.00	0/838	1.15	0/1131
10	J	0.93	0/832	1.14	1/1119 (0.1%)
11	K	0.95	0/776	1.08	0/1038
12	L	0.94	0/872	1.18	2/1176 (0.2%)
13	M	0.95	0/752	1.11	0/1006
14	N	1.01	0/864	1.21	0/1175
15	O	0.97	0/1012	1.18	0/1358
16	P	3.15	6/538 (1.1%)	2.40	20/746 (2.7%)
17	Q	0.50	2/1009 (0.2%)	1.24	9/1392 (0.6%)
18	R	1.42	1/738 (0.1%)	1.72	4/1025 (0.4%)
All	All	1.06	44/121300 (0.0%)	1.53	254/164153 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	B	0	11
3	C	0	1
4	D	0	1
7	G	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	P	0	2
All	All	0	31

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	59	THR	C-N	-63.98	0.44	1.33
1	A	1067	PRO	N-CD	51.37	2.19	1.47
16	P	62	LYS	C-N	-49.90	0.63	1.33
16	P	15	SER	C-N	35.27	1.81	1.34
18	R	82	ALA	C-N	30.48	1.71	1.33

The worst 5 of 254 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1171	ILE	CA-C-N	-61.26	4.53	121.54
1	A	1171	ILE	C-N-CA	-61.26	4.53	121.54
2	B	59	THR	O-C-N	-50.05	59.78	122.34
2	B	49	PHE	O-C-N	-38.44	78.07	123.04
2	B	137	LEU	N-CA-C	31.89	152.77	113.23

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1171	ILE	Peptide,Mainchain
1	A	121	GLY	Mainchain
1	A	1649	ALA	Mainchain
2	B	25	GLN	Peptide
2	B	49	PHE	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33975	0	32379	2250	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	34751	0	33289	2401	0
3	C	30427	0	29352	1265	0
4	D	4680	0	4511	1087	0
5	E	4440	0	4311	928	0
6	F	996	0	1019	266	0
7	G	1024	0	883	193	0
8	H	750	0	734	226	0
9	I	827	0	826	297	0
10	J	807	0	772	271	0
11	K	754	0	716	125	0
12	L	855	0	854	214	0
13	M	735	0	738	196	0
14	N	852	0	799	197	0
15	O	994	0	1017	310	0
16	P	541	0	217	58	0
17	Q	1006	0	512	53	0
18	R	739	156	339	46	0
19	A	54	0	23	32	0
19	B	54	0	24	18	0
19	C	54	0	22	32	0
20	A	31	0	12	10	0
20	B	31	0	12	43	0
20	C	31	0	12	2	0
21	A	3	0	0	2	0
21	B	3	0	0	0	0
21	C	3	0	0	0	0
All	All	119417	156	113373	8721	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

The worst 5 of 8721 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:86:CYS:SG	11:K:61:VAL:HG22	1.24	1.72
1:A:3235:TYR:CE2	1:A:3269:LEU:HD13	1.25	1.71
3:C:196:PRO:HA	3:C:239:TRP:CZ2	1.23	1.67
2:B:3118:TYR:CE2	2:B:3452:LEU:HA	1.25	1.64
4:D:170:THR:CG2	13:M:66:ILE:CG1	1.74	1.64

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4391/4615 (95%)	4176 (95%)	190 (4%)	25 (1%)	21	58
2	B	4498/4588 (98%)	4258 (95%)	203 (4%)	37 (1%)	16	53
3	C	3923/3947 (99%)	3698 (94%)	202 (5%)	23 (1%)	21	58
4	D	569/595 (96%)	546 (96%)	16 (3%)	7 (1%)	10	43
5	E	551/557 (99%)	531 (96%)	18 (3%)	2 (0%)	30	67
6	F	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
7	G	147/151 (97%)	134 (91%)	7 (5%)	6 (4%)	2	18
8	H	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
9	I	104/106 (98%)	100 (96%)	3 (3%)	1 (1%)	12	47
10	J	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
11	K	88/90 (98%)	85 (97%)	3 (3%)	0	100	100
12	L	109/111 (98%)	104 (95%)	4 (4%)	1 (1%)	14	49
13	M	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
14	N	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
15	O	118/120 (98%)	112 (95%)	4 (3%)	2 (2%)	7	35
16	P	103/112 (92%)	90 (87%)	7 (7%)	6 (6%)	1	14
17	Q	190/192 (99%)	174 (92%)	13 (7%)	3 (2%)	7	37
18	R	148/150 (99%)	121 (82%)	19 (13%)	8 (5%)	1	15
All	All	15444/15849 (97%)	14615 (95%)	708 (5%)	121 (1%)	18	53

5 of 121 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	PRO
1	A	125	PRO
1	A	127	THR
1	A	151	ILE

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Mol	Chain	Res	Type
1	A	1171	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3430/4191 (82%)	3329 (97%)	101 (3%)	37	58
2	B	3525/4135 (85%)	3437 (98%)	88 (2%)	42	62
3	C	3139/3505 (90%)	3084 (98%)	55 (2%)	51	67
4	D	511/545 (94%)	497 (97%)	14 (3%)	39	59
5	E	488/496 (98%)	469 (96%)	19 (4%)	28	50
6	F	105/105 (100%)	103 (98%)	2 (2%)	50	66
7	G	86/141 (61%)	86 (100%)	0	100	100
8	H	82/82 (100%)	81 (99%)	1 (1%)	63	73
9	I	91/91 (100%)	89 (98%)	2 (2%)	45	64
10	J	82/82 (100%)	81 (99%)	1 (1%)	63	73
11	K	80/80 (100%)	78 (98%)	2 (2%)	42	62
12	L	90/99 (91%)	87 (97%)	3 (3%)	33	55
13	M	78/78 (100%)	78 (100%)	0	100	100
14	N	84/101 (83%)	82 (98%)	2 (2%)	43	63
15	O	108/108 (100%)	107 (99%)	1 (1%)	70	76
17	Q	11/176 (6%)	11 (100%)	0	100	100
All	All	11990/14015 (86%)	11699 (98%)	291 (2%)	43	63

5 of 291 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	3405	ARG
12	L	66	GLU
3	C	3918	VAL
5	E	139	GLU

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Mol	Chain	Res	Type
1	A	4504	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 274 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	512	HIS
5	E	237	ASN
10	J	63	HIS
2	B	1135	HIS
2	B	1079	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	ATP	B	5601	21	32,33,33	0.54	0	48,52,52	0.62	0
19	ADP	A	4901	21	28,29,29	1.38	4 (14%)	43,45,45	1.84	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	ATP	C	4201	21	32,33,33	0.49	0	48,52,52	0.65	0
20	ATP	A	4801	21	32,33,33	1.31	4 (12%)	48,52,52	1.73	10 (20%)
19	ADP	C	4702	21	28,29,29	0.50	0	43,45,45	0.83	1 (2%)
19	ADP	C	4703	21	28,29,29	0.46	0	43,45,45	0.61	0
19	ADP	A	4701	21	28,29,29	1.40	5 (17%)	43,45,45	1.87	9 (20%)
19	ADP	B	5602	21	28,29,29	0.46	0	43,45,45	0.47	0
19	ADP	B	5501	21	28,29,29	0.48	0	43,45,45	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	ATP	B	5601	21	-	2/22/38/38	0/3/3/3
19	ADP	A	4901	21	-	6/16/32/32	0/3/3/3
20	ATP	C	4201	21	-	3/22/38/38	0/3/3/3
20	ATP	A	4801	21	-	3/22/38/38	0/3/3/3
19	ADP	C	4702	21	-	7/16/32/32	0/3/3/3
19	ADP	C	4703	21	-	4/16/32/32	0/3/3/3
19	ADP	A	4701	21	-	8/16/32/32	0/3/3/3
19	ADP	B	5602	21	-	1/16/32/32	0/3/3/3
19	ADP	B	5501	21	-	3/16/32/32	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	4901	ADP	C5-C4	4.52	1.47	1.39
19	A	4701	ADP	C5-C4	4.39	1.46	1.39
20	A	4801	ATP	C5-C4	4.10	1.46	1.39
19	A	4901	ADP	C5-C6	2.77	1.48	1.41
20	A	4801	ATP	C5-N7	-2.68	1.34	1.39

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	4701	ADP	C5-C4-N3	-6.24	118.13	126.72
19	A	4901	ADP	C5-C4-N3	-5.79	118.74	126.72
20	A	4801	ATP	C5-C4-N3	-5.74	118.81	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	4901	ADP	N3-C4-N9	4.63	135.05	127.17
20	A	4801	ATP	N3-C4-N9	4.58	134.96	127.17

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

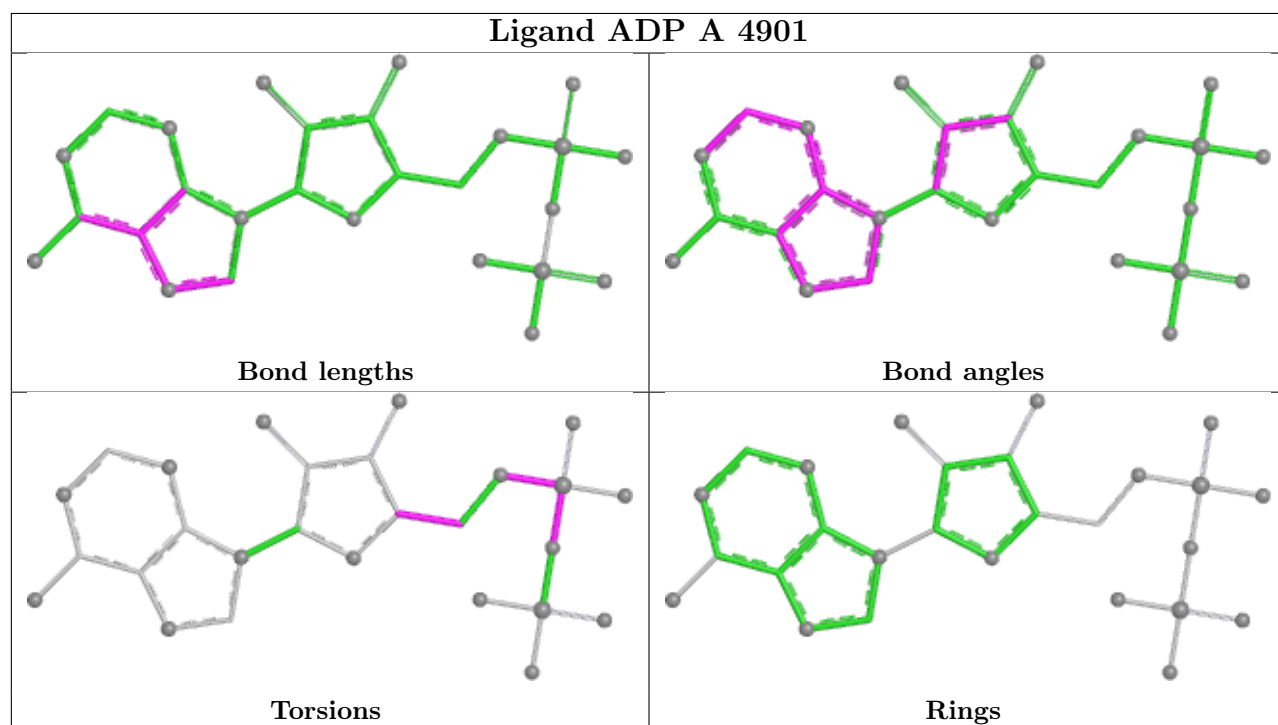
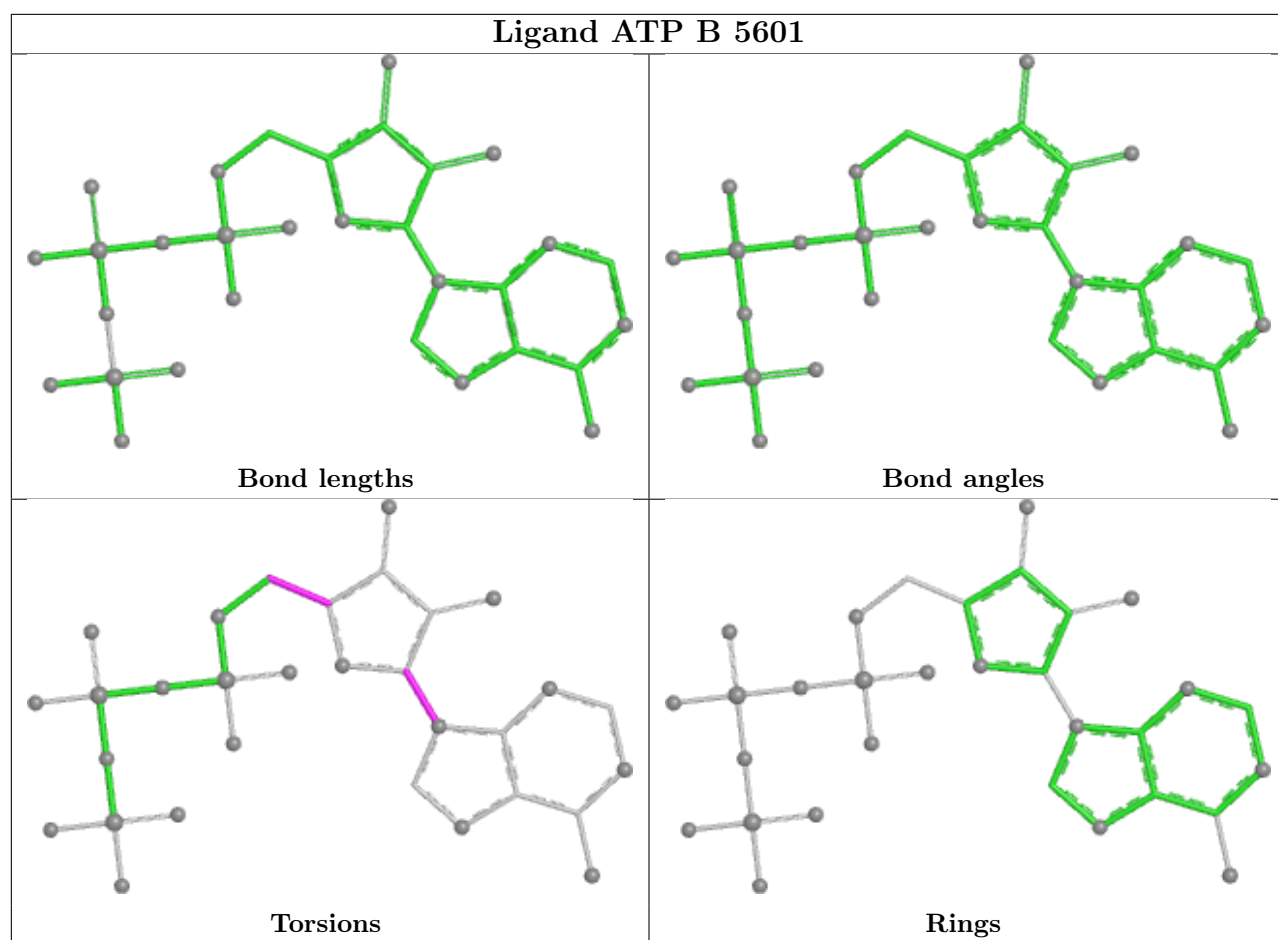
Mol	Chain	Res	Type	Atoms
19	A	4701	ADP	PB-O3A-PA-O5'
19	A	4701	ADP	C5'-O5'-PA-O1A
19	A	4701	ADP	C5'-O5'-PA-O2A
19	A	4701	ADP	C5'-O5'-PA-O3A
19	A	4901	ADP	PB-O3A-PA-O5'

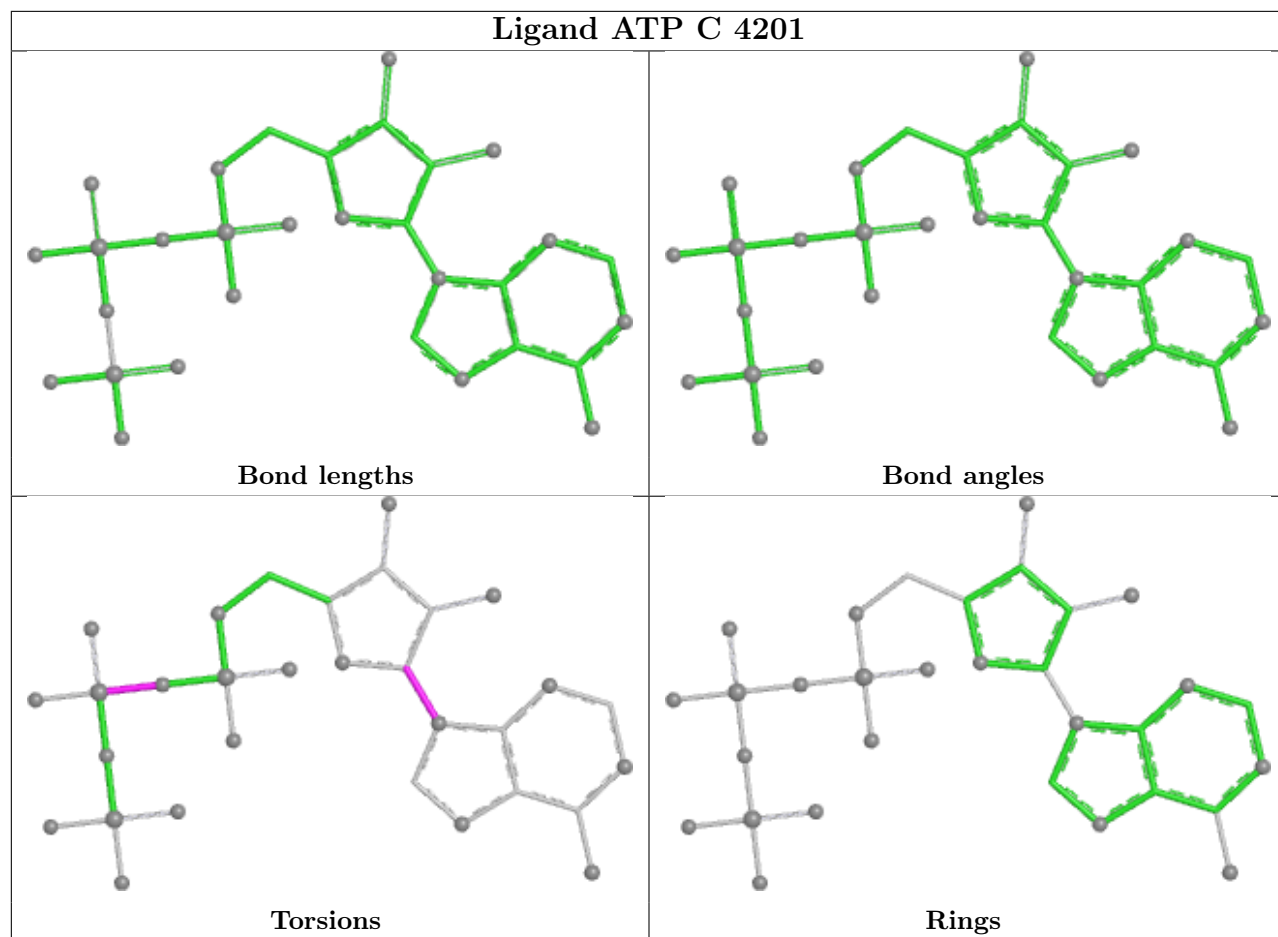
There are no ring outliers.

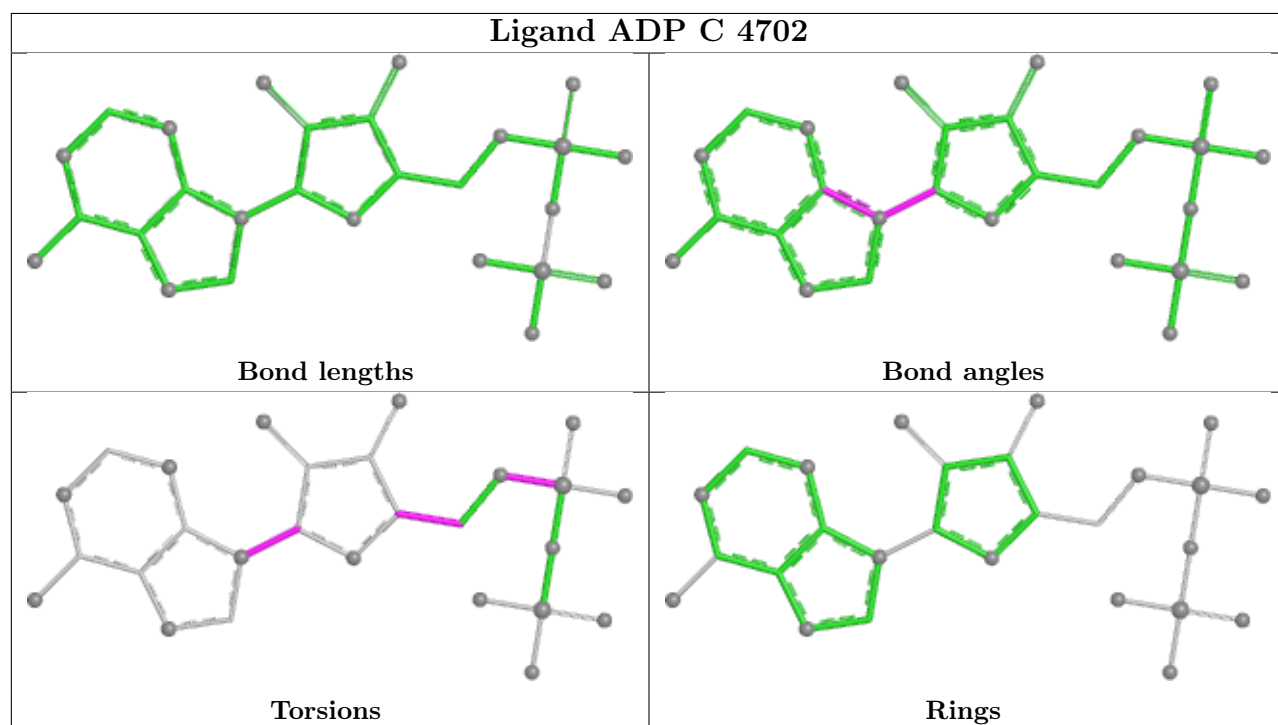
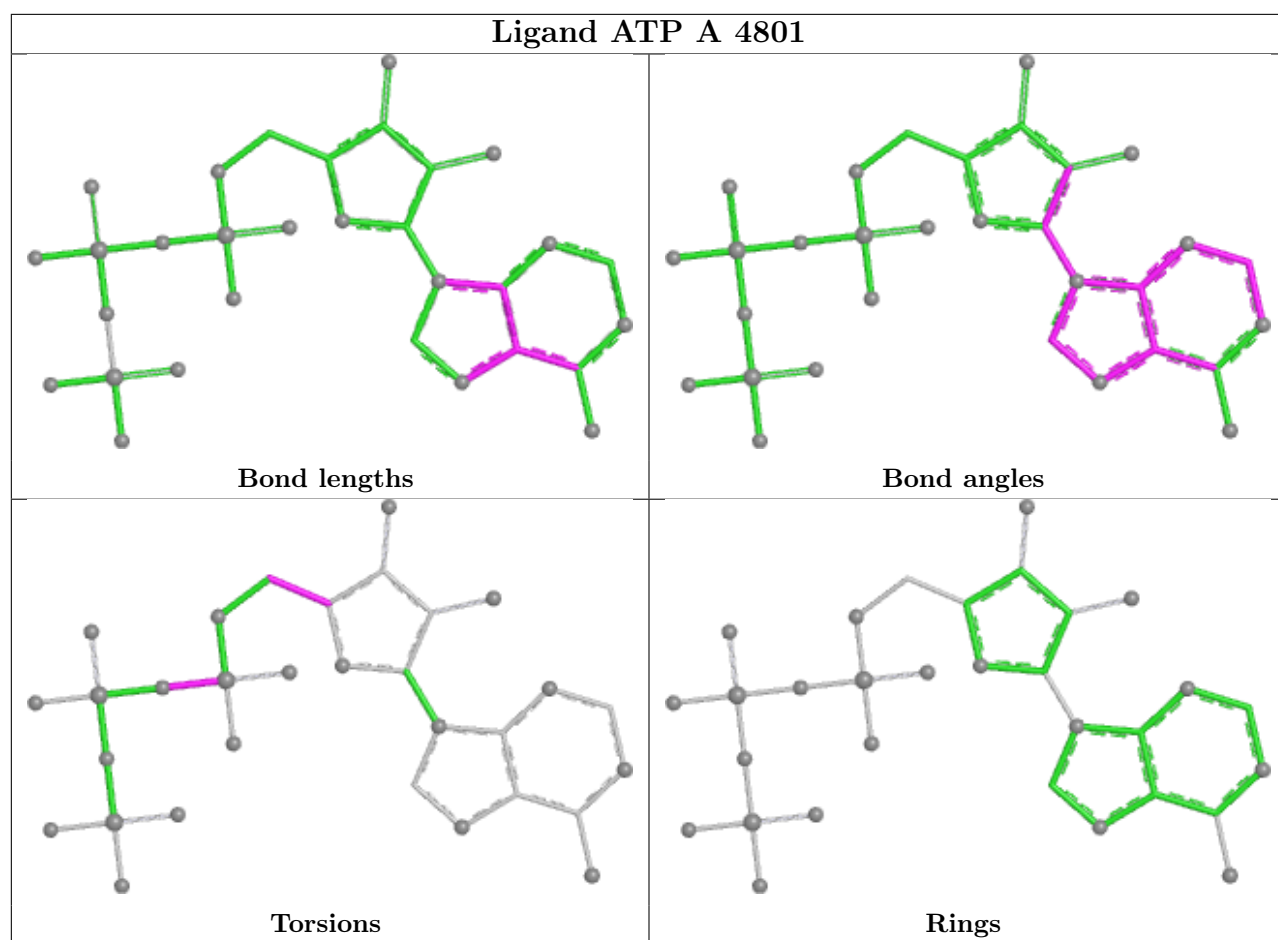
9 monomers are involved in 137 short contacts:

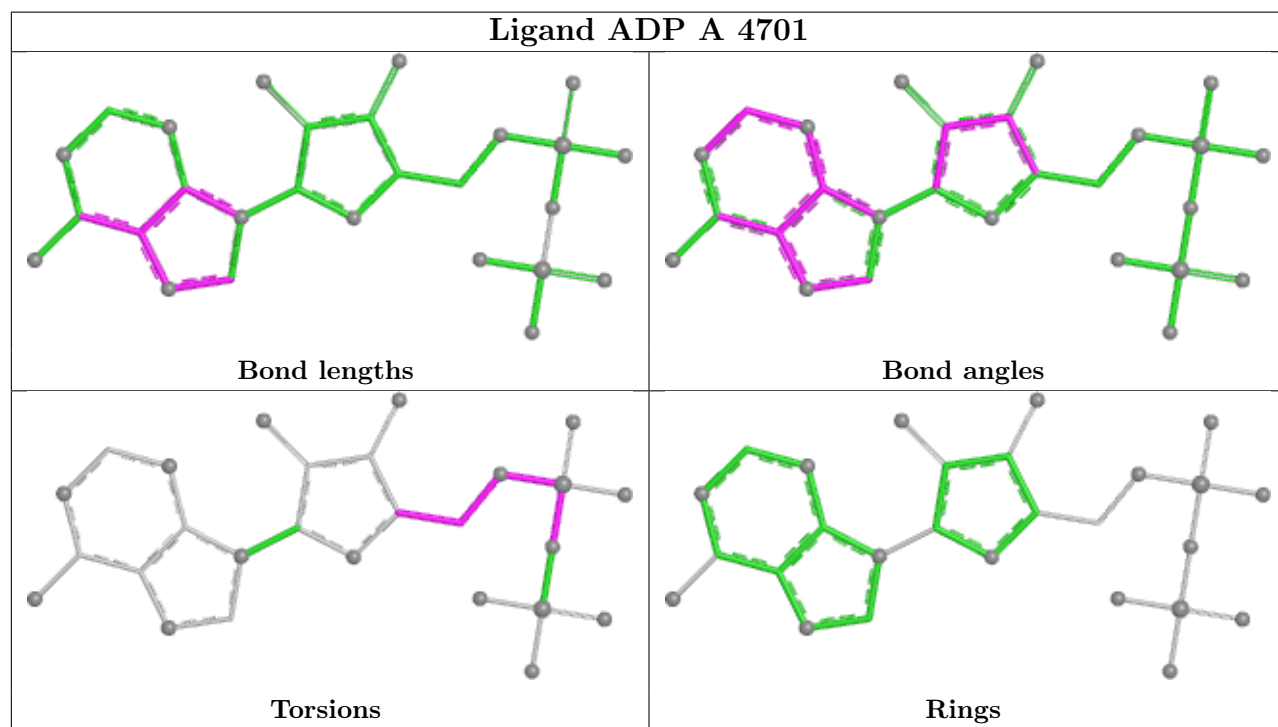
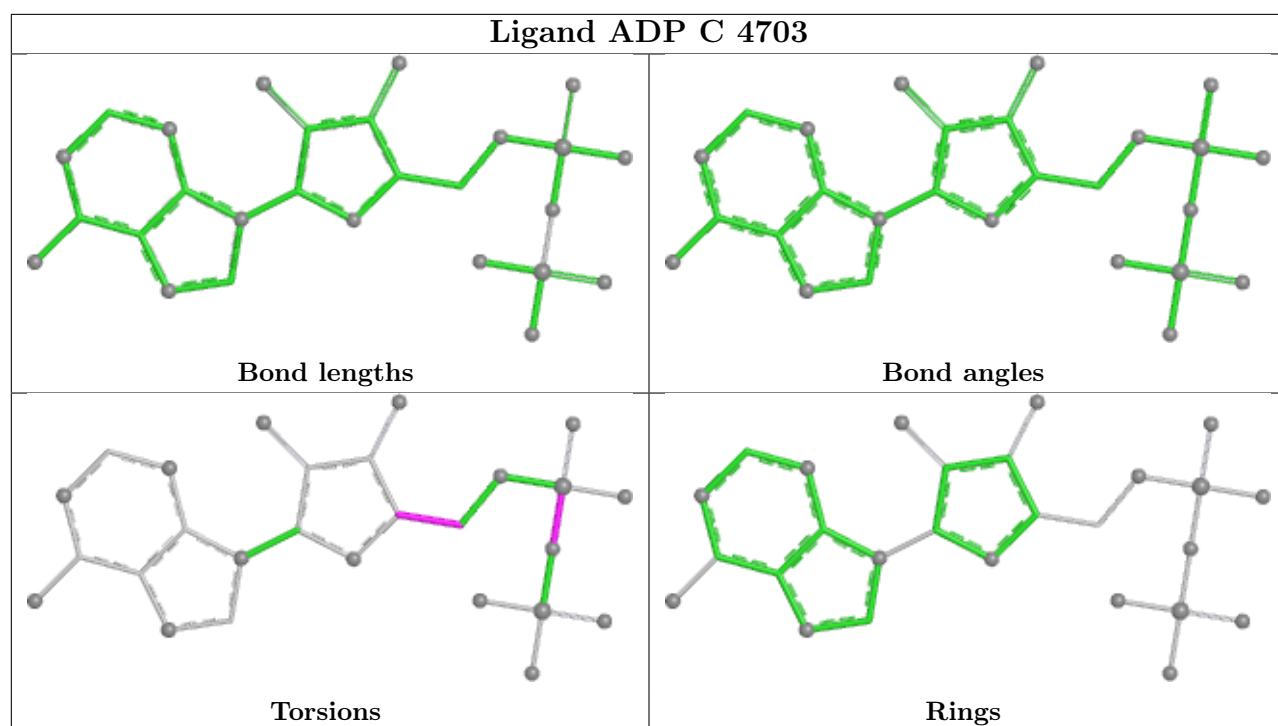
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	5601	ATP	43	0
19	A	4901	ADP	19	0
20	C	4201	ATP	2	0
20	A	4801	ATP	10	0
19	C	4702	ADP	25	0
19	C	4703	ADP	7	0
19	A	4701	ADP	13	0
19	B	5602	ADP	2	0
19	B	5501	ADP	16	0

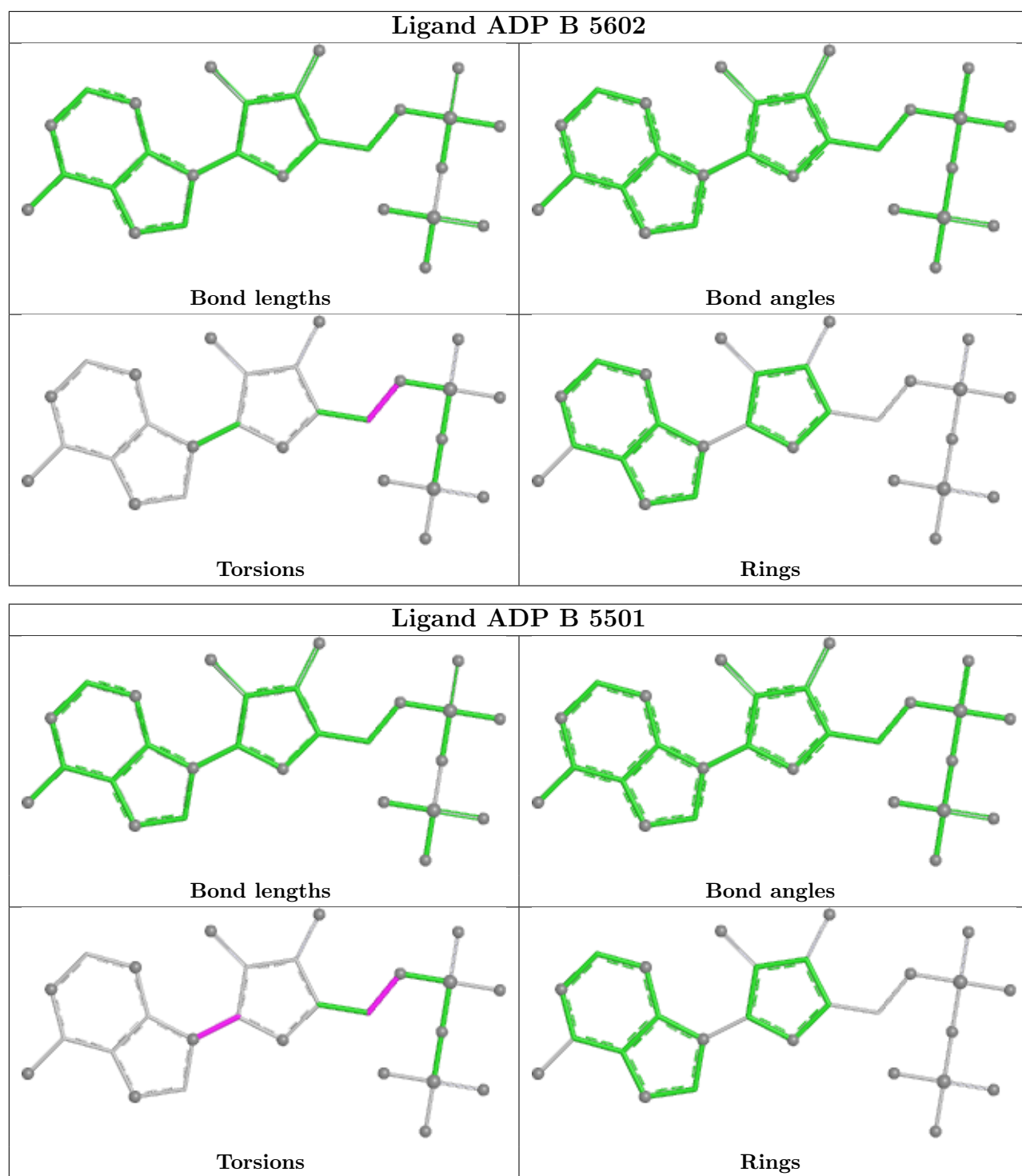
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	12
3	C	11
2	B	11
16	P	4
4	D	2
7	G	1
18	R	1

The worst 5 of 42 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3277:MET	C	3380:MET	N	42.67
1	A	1235:PRO	C	1246:MET	N	14.08
1	C	809:ARG	C	818:ILE	N	13.93
1	C	449:TYR	C	452:ASN	N	13.33
1	C	665:ILE	C	670:SER	N	11.69

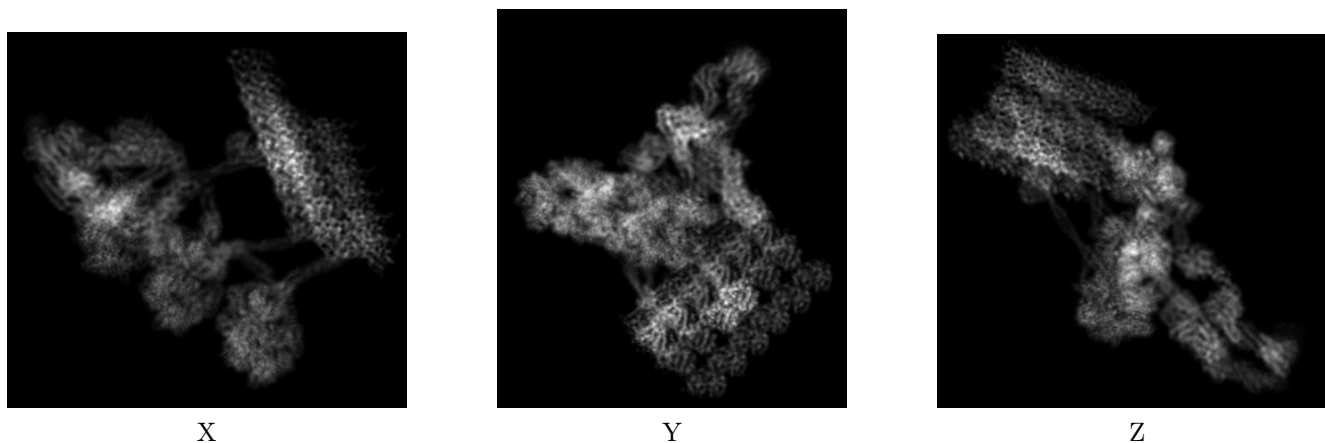
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22679. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

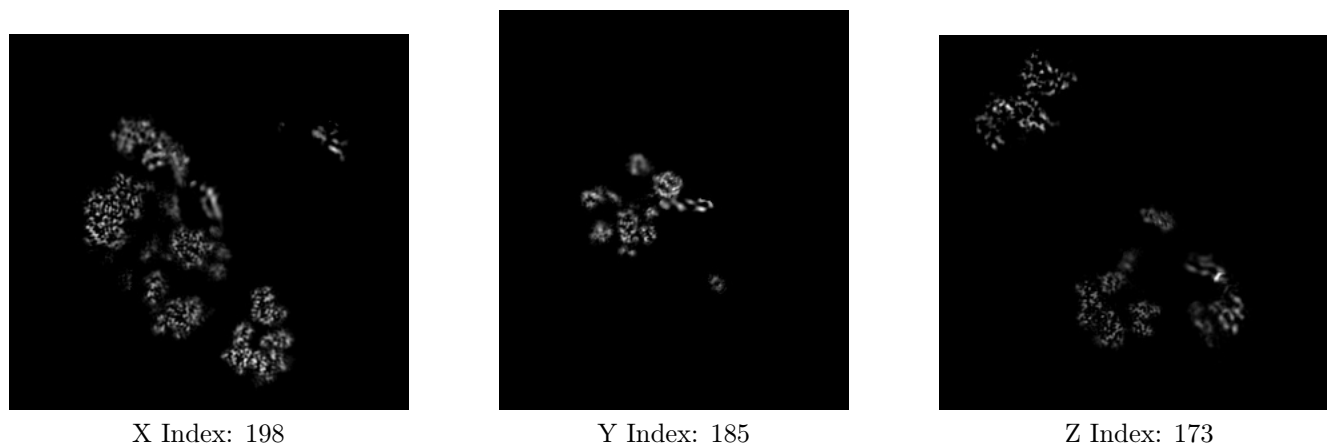
6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 97



Y Index: 249

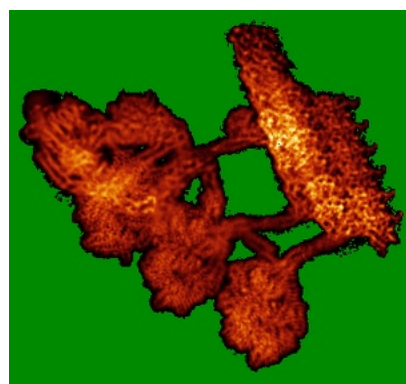


Z Index: 228

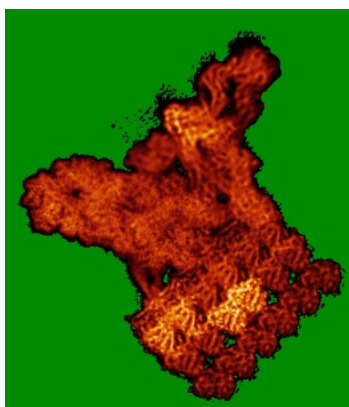
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

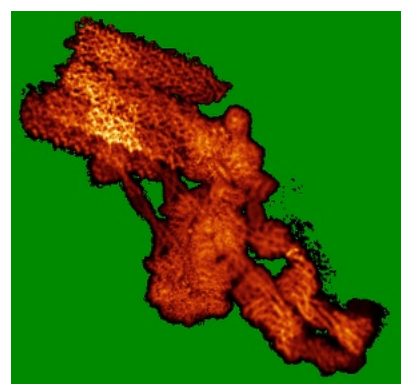
6.4.1 Primary map



X



Y

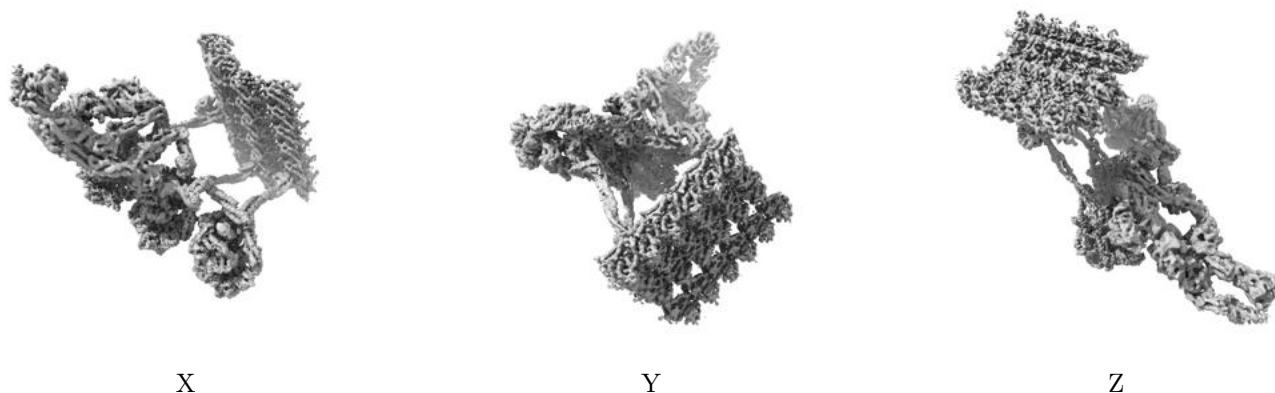


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

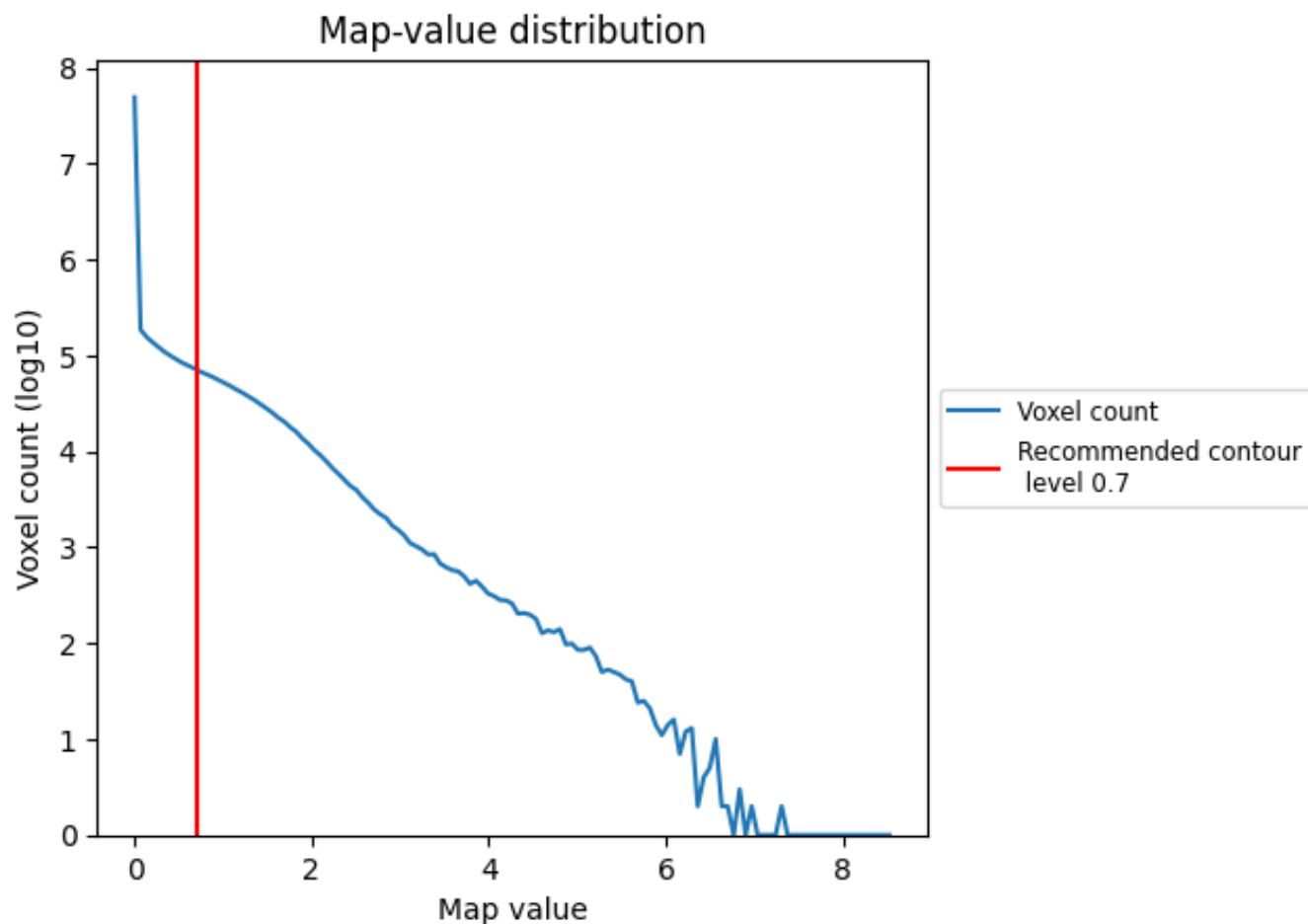
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

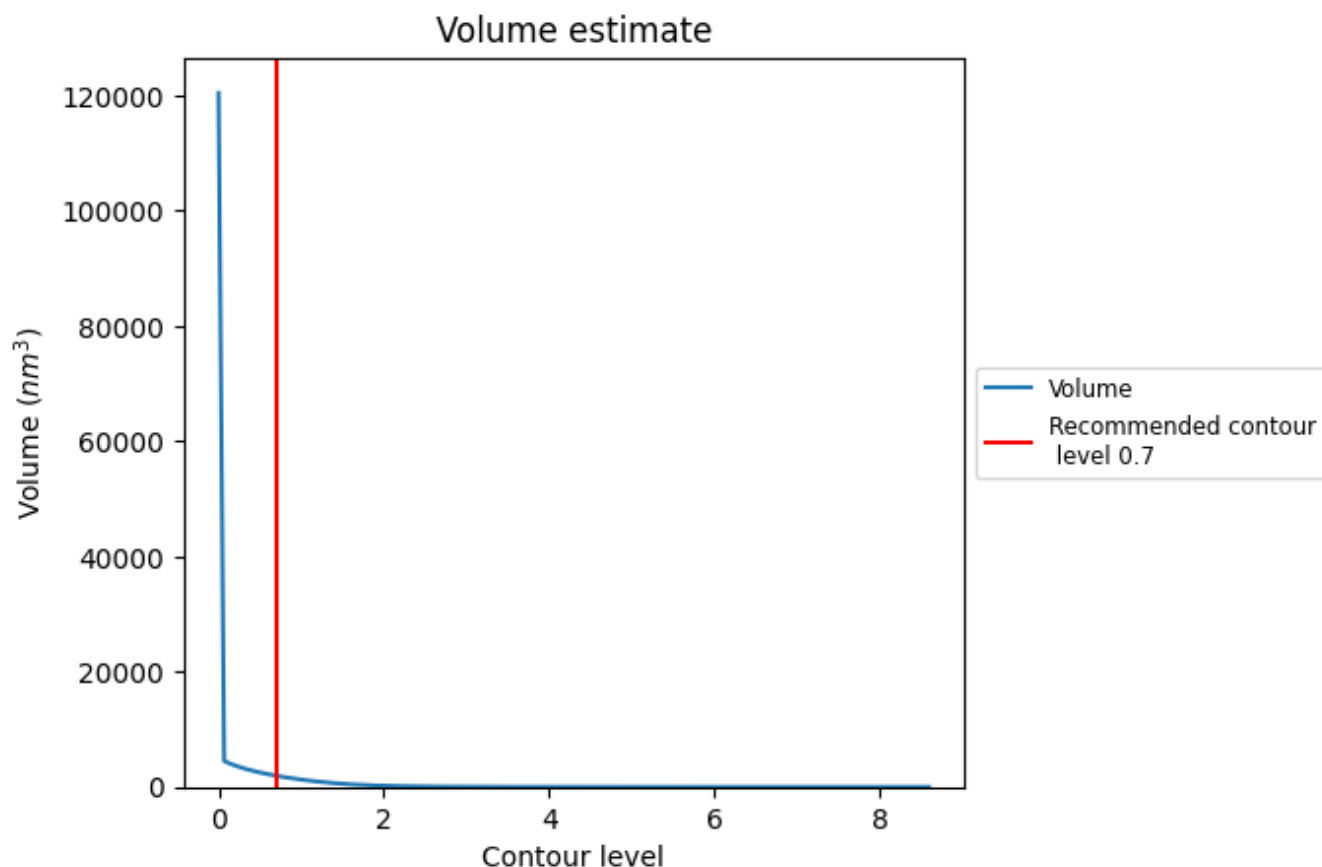
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1940 nm³; this corresponds to an approximate mass of 1753 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

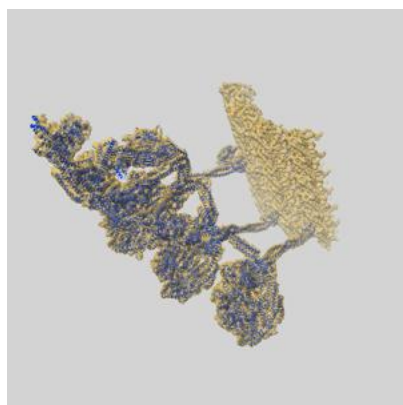
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

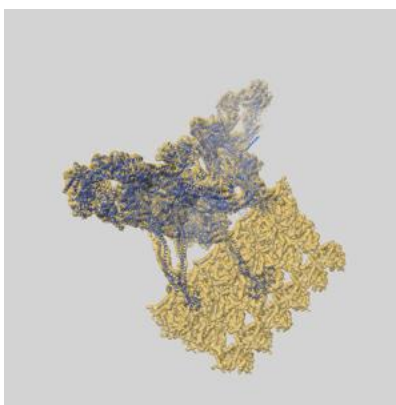
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22679 and PDB model 7K5B. Per-residue inclusion information can be found in section [3](#) on page [9](#).

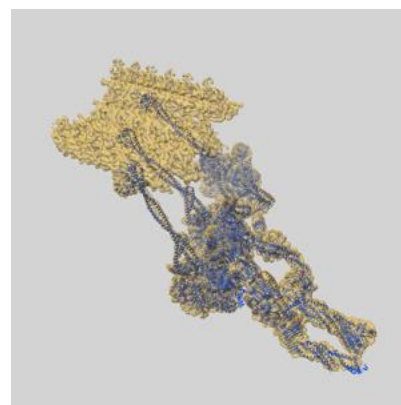
9.1 Map-model overlay [i](#)



X



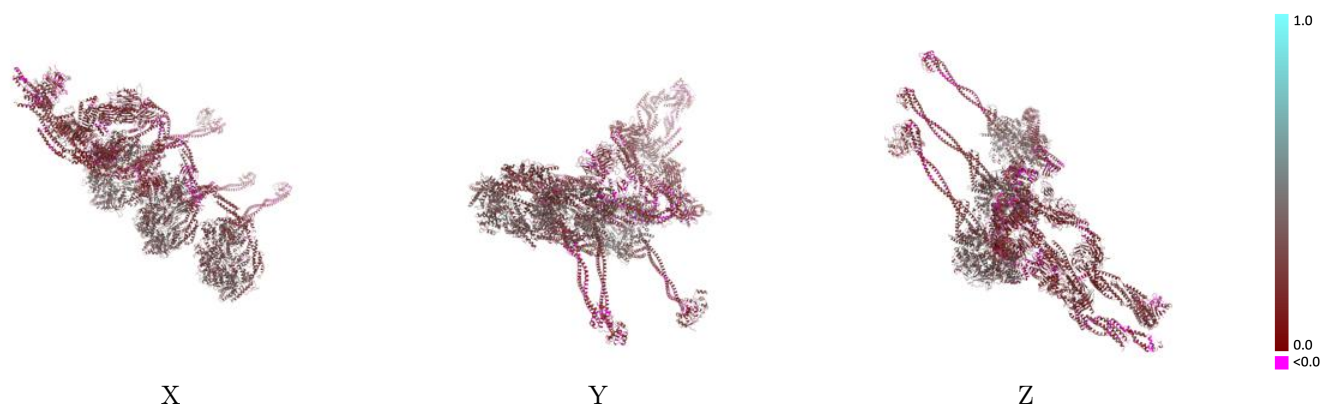
Y



Z

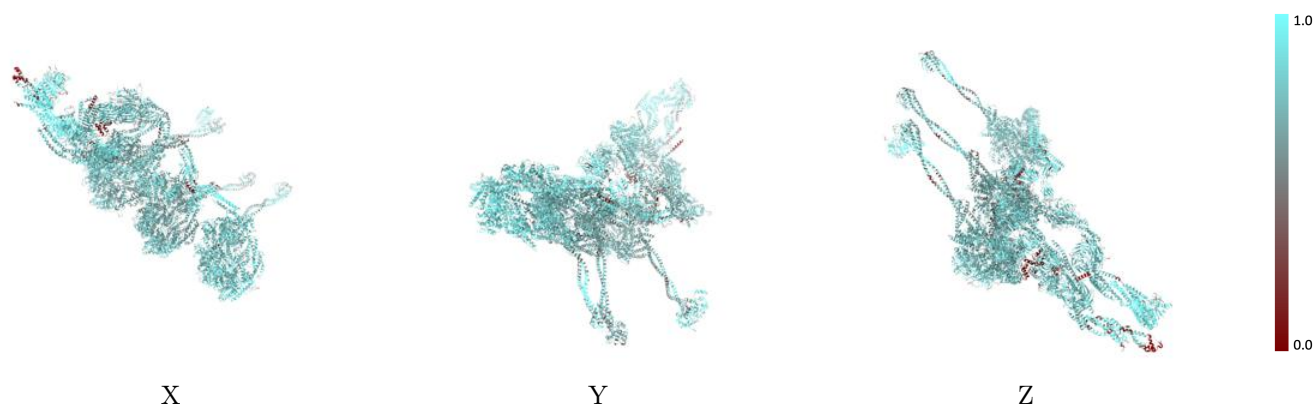
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



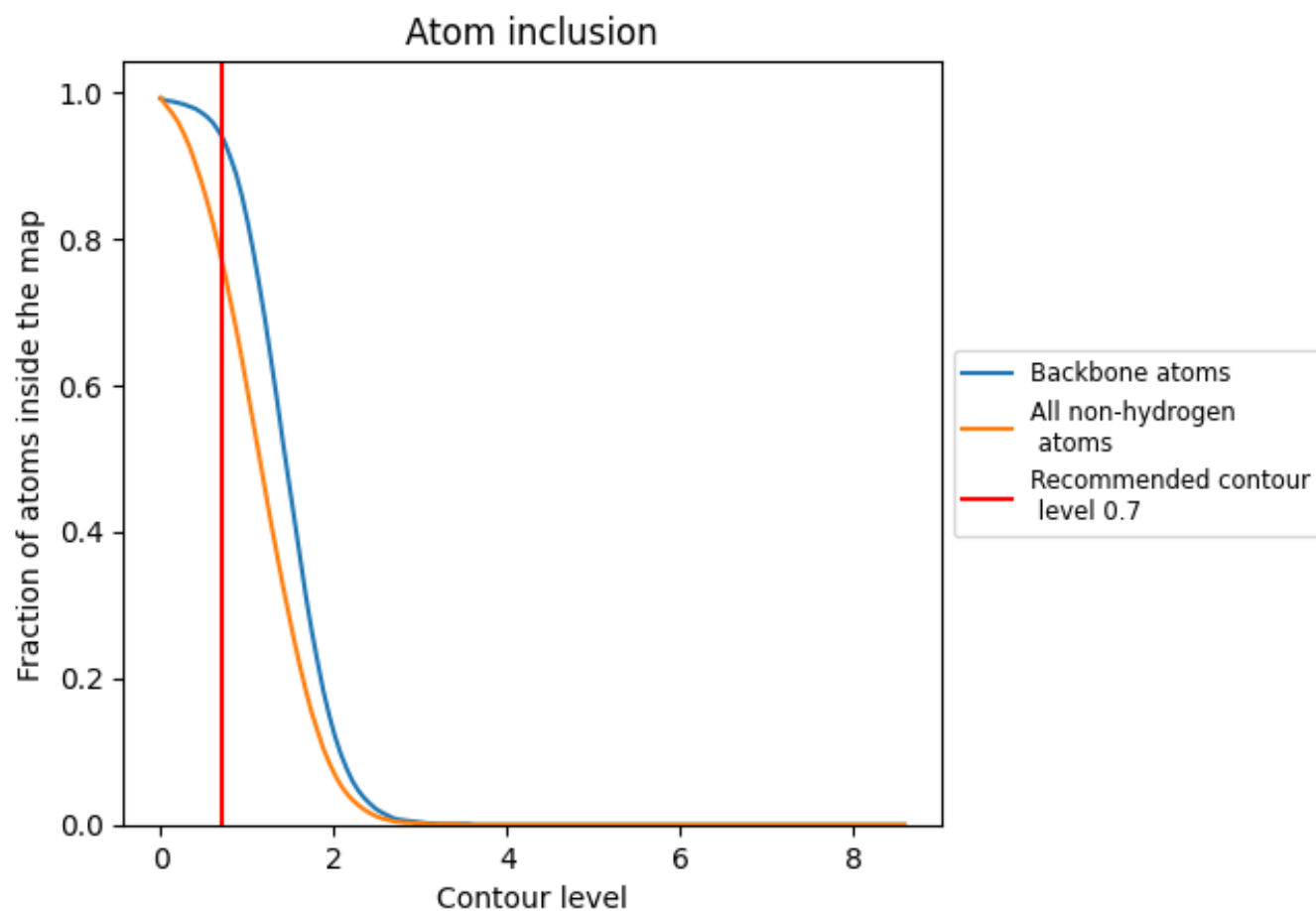
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7740	 0.2640
A	 0.7590	 0.2830
B	 0.7570	 0.2730
C	 0.8180	 0.2860
D	 0.8030	 0.2060
E	 0.8280	 0.2060
F	 0.7010	 0.1850
G	 0.6180	 0.1440
H	 0.7740	 0.1860
I	 0.8050	 0.1730
J	 0.7950	 0.1850
K	 0.8070	 0.1780
L	 0.6570	 0.1780
M	 0.7680	 0.1590
N	 0.7670	 0.1640
O	 0.7500	 0.1440
P	 0.8910	 0.1510
Q	 0.8490	 0.2450
R	 0.0270	 -0.0320

